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Applications of point group symmetries in light nuclei

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Applications of point group symmetries in light nuclei

by

Paul Stephen Hauge

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I. INTRODUCTION

In 1949 Jensen (1) and Mayer (2) independently discovered that the addition of a large spin-orbit term to a shell model potential could explain all of the observed nuclear shell closures. Since that time the model has met with such spectacular success in describing a multitude of nuclear phenomena, that it is today considered as the fundamental basis for nearly all nuclear calculations. The assumptions of the model are too extreme to yield a final quantitative analysis of nuclear properties, so for the past twenty years, many theorists have concentrated their attention towards performing Hartree-Fock calculations using the shell model wavefunctions as a zeroth-order basis. Unfortunately, such realistic calculations have been prohibitive unless one (a) works with nuclei near closed shells, (b) makes drastic assumptions concerning the truncation of the basis states, or (c) limits his computations to the ground state energy level. In addition, many physicists have found these calculations quite unpleasant, since much of the physics is lost or hidden in the numerical work.

The inherent difficulties of these microscopic calculations were well realized in the early 1950's; consequently many physicists searched for modifications of the shell model which would explicate the levels in a simpler way. Most of the nuclei away from closed shells were known to exhibit definite collective properties, so several attempts were made to unify these collective and single-particle features. Some of these "unified" models were found to be very successful for large mass regions. For example, various unified models which assume the nucleus to have static or dynamic deformations are now thought to describe the basic dynamics of nearly all
heavy nuclei in the mass region $150 < A < 180$ and $A < 220$ \(^{(3)}\). The deformations are usually considered to be prolate and have axial symmetry. However, one model assumes further deformation by compressing the nucleus along one of the axes in the equatorial plane.

Unfortunately, no conclusive model has yet been found for light nuclei ($4 < A < 40$). This is very discouraging, since such a model would dictate how one could best proceed with realistic calculations. Extended shell model calculations can predict many properties of these nuclei; but other observables are not well described and show definite collective features \(^{(4)}\). In particular, the experimental ground state quadrupole moments are usually several times larger than the shell model predictions, and many electric quadrupole and octopole transitions are one to two orders of magnitude larger than the single-particle estimates. The various forms of unified models mentioned earlier are natural candidates for explaining these collective features. However, in practice they are found to describe only a few of the excited states for most nuclei in this region \(^{(4)}\). This is not too surprising because one would not expect the limited number of nucleons present in light nuclei to be able to consistently produce the simple deformations observed in heavier mass regions. For light nuclei, more complicated shapes may be needed.

One other collective model exists for light nuclei which may be able to solve this difficulty. Commonly referred to as the alpha model, it assumes that the nucleons cluster into temporary or permanent alpha particles. For reasons which will become evident in Section B, the alpha model has so far not been fully developed. Therefore, in the present work we will consider two forms of the alpha model and test their validity on the observed
properties of many light nuclei. In particular, we will assume the alpha clusters to be of such long duration that they can form permanent "molecular" alpha structures of a definite point group symmetry. The imposed symmetry will then be shown to have a direct influence on the observed properties of low-lying energy levels.

The rest of Chapter I deals with general information concerning the alpha model. In Section A we list some of the experimental evidence now available which supports alpha clustering in light nuclei, and a historical review of the alpha model is given in Section B. At that time, it will be noted that the alpha model actually includes several different types of calculations. In particular, we shall distinguish between "α-particle" and "α-cluster" models. The former will denote only those models which assume that the alpha particles are permanent entities of a nucleus; the latter is reserved for more realistic models which consider methods of enhancing four-body correlations among the individual nucleons. These different forms will be mentioned briefly in chronological order, but will not be described in detail until later chapters.

In Chapter II, we shall be concerned only with the development of the classical α-particle (CAP) model and its application to numerous light \(A=4N\) nuclei (where \(A\) is the number of nucleons and \(N\) is an integer). The CAP model is the simplest of all possible alpha-particle models and assumes that light \(A=4N\) nuclei are composed entirely of permanent alpha particles arranged in a definite molecular structure. Such an assumption is naturally too extreme to be very realistic; but the model is completely phenomenological anyway, so it may still be a valid approximation. The Hamiltonian and wavefunction for the CAP model are derived in Section A. As has already
been implied, the most important feature of the CAP model is that the spatial symmetry of the assumed \( \alpha \)-structure dictates the spins and parities of the low-lying levels; this aspect is described in Sections B, C, and D. The theory for calculating the electron scattering cross sections and reduced transition matrix elements is then developed in Sections E and F. Then, in Section G, we review the past work of the CAP model for \( A=4N \) nuclei in the \( 1p \) shell, and show that the model works quite well but is incapable of predicting some of the observed low-lying transitions. By noting these discrepancies we are then able to give some further qualitative arguments concerning the validity of the CAP model for other \( A=4N \) nuclei. The conclusions drawn in Section G will be quite favorable for the CAP model. Therefore in Section H, we consider various \( \alpha \)-structures for all \( A=4N \) nuclei in the \( 2s-1d \) shell, and assume the physical structure to be the one that yields theoretical predictions in best agreement with experiment. Some general conclusions concerning the charge and mass distributions are then given in Section I for many of the nuclei considered. Finally, in Section J we compare the results of the CAP model with other models that have been considered for these nuclei.

In Chapter III, we digress from the alpha particle model and review the basic theory of other well-known collective and unified models. There has been some confusion in the literature as to the distinction between collective and unified models, and some authors use the terms interchangeably. In the present work, we reserve the name "collective" for models of even-even nuclei where all the nucleons are presumed assimilated in the deformed core. We shall not refer to a model as being unified until it has been extended to include extra-core nucleons. The purpose of this chapter is to briefly
review the theory of the other collective models (for even-even nuclei), so that some parallelisms between these models and the CAP model can be made. In particular, it will be shown in Section D that the theories for the symmetric and asymmetric collective rotors are analogous to two special cases of the CAP model. Then in Section E, the theory will be reviewed for extending the collective symmetric rotor to odd-A nuclei. With this accomplished it is finally inferred that the theory for the unified symmetric and asymmetric rotors might be generalized into an $\alpha$-particle model appropriate for light odd-A nuclei.

In Chapter IV, we develop this supposition into a theory and formulate the unified $\alpha$-particle (UAP) model for light $A=4N+1$ nuclei. The necessary theory is developed in the first three sections. Then in Section D, we will compare the theoretical predictions to the experimental data available for the $A=9$ and 13 mass systems. Finally, in Section E, we again collate the results of the UAP model with those of other models which have been considered for nuclei in this region.

Finally, in Chapter V, we review the principle contributions of the present work as well as present some future problems that need to be solved within the framework of the alpha model.

A. Evidence for Alpha Clustering in Nuclei

There are several valid reasons for assuming that alpha correlations may be enhanced in many nuclei. Four of the more common ones are the following:

1. Many nuclei heavier than $^{208}$Pb decay by alpha emission indicating that alpha clusters are present at least part of the time in heavy nuclei.
This information was well-known in the early 1900's and led directly to the formulation of the alpha model in 1930 (5).

2. If one constructs a curve of the neutron binding energy versus mass number $A$ for nuclei having a minimum neutron excess $(N-Z)$, one obtains the saw-toothed curve shown in Figure 1.1. This curve was first noted by Baz (6) in 1955, and shows that alpha clustering may be prevalent in all nuclei up through $^{40}\text{Ca}$.

3. All $A=4N$ nuclei with mass less than or equal to $^{40}\text{Ca}$ have alpha thresholds at lower energy than their nucleon thresholds as shown in Figure 1.2. Since the nucleons are more tightly bound than the alpha particles, this fact could imply that the nucleons are bound inside internal alpha clusters.

4. Alpha correlations arise naturally from the single-particle shell-model states due to the Pauli-exclusion principle. Wheeler (7) first recognized this fact in 1937 and explained the correlation tendencies by using $^{16}\text{O}$ as an example. Using Wheeler's example, as well as his notation, we write the many-particle zeroth-order Hartree-Fock ground state for $^{16}\text{O}$ as

$$
\Psi(i_1, \ldots, i_{16}) = \begin{vmatrix}
(s a | 1) & (s b | 1) & \cdots & (P_z d | 1) \\
(s a | 2) & & \cdots & \\
& \cdots & \cdots & \\
& \cdots & \cdots & \\
(s a | 16) & \cdots & \cdots & (P_z d | 16)
\end{vmatrix}, \quad (1.1)
$$

where $a, b, c, d$ represent the four spin and isotopic spin states of a nucleon, and $s, p_x, p_y, p_z$ represent the lowest-lying single particle orbital
Figure 1.1. Plot of neutron binding energy versus mass of nuclei with a minimum neutron excess (N-Z).

Figure 1.2. The lower, middle, and top curves describe the binding energy of the alpha particle, proton, and neutron respectively in light $A=4N$ nuclei.
states of the nucleus. We now add and subtract rows and columns without changing the value of the determinant to obtain

$$\Psi' (l_1, \ldots, l_6) = \begin{vmatrix} (x \alpha l_1) & \ldots & (x \alpha l_6) \\ \ldots & \ldots & \ldots \\ (x \alpha l_1) & \ldots & (x \alpha l_6) \end{vmatrix},$$

(1.2)

where the new orbital states are defined by the following orthogonal transformations

$$\langle x l_1 \rangle = \frac{1}{2} [ (s l_1) + (P_x l_1) + (P_y l_1) + (P_z l_1) ]$$

$$\langle x l_2 \rangle = \frac{1}{2} [ (s l_2) + (P_x l_2) - (P_y l_2) - (P_z l_2) ]$$

$$\langle x l_3 \rangle = \frac{1}{2} [ (s l_3) - (P_x l_3) + (P_y l_3) - (P_z l_3) ]$$

$$\langle x l_4 \rangle = \frac{1}{2} [ (s l_4) - (P_x l_4) - (P_y l_4) + (P_z l_4) ]$$

(1.3)

The two wavefunctions in Equations 1.1 and 1.2 are identical, but the latter is rewritten in order to demonstrate that there exists a large probability of finding the building material for an alpha particle near each vertex of a tetrahedron. Presumably, the short-range nuclear forces should grasp this opportunity to form alpha clusters, and such cluster correlations should be realized from Hartree-Fock calculations. In recent years, density plots of HF ground states have been made for several light nuclei and they do seem to indicate some degree of alpha correlations (8).

The preceding list of four statements is by no means complete; its purpose is simply to present a few of the reasons why many people now believe
there is some validity to the alpha model. Much of the other evidence, such as spins and parities of low-lying levels, are dependent on the assumed shape of the nucleus and will be considered in later chapters.

B. Historical Review of the Alpha Model

The alpha model was first proposed by Gamow (5) in 1930 as a natural extension to his successful investigation of alpha decay two years earlier. In what is now a classic paper, he proceeded to estimate the mass defects of nuclei by assuming they were composed almost entirely of alpha particles. The neutron was not discovered until 1932, so for most nuclei he needed to add a small number of protons and "nuclear electrons" to produce the desired charge and mass.

Naturally, the discovery of the neutron made this paper obsolete, and the alpha model was discarded in favor of the shell model which was advanced by a number of physicists beginning in 1934 (9). However, many physicists intuitively felt that the nuclear levels were more like those of a molecule or a liquid drop rather than like the electronic states of an atom. They were especially critical of the central field approximation needed for the shell model; it was valid in the atomic case, but probably did not have too much meaning for light nuclei (10). In 1936, this feeling was augmented by Bohr who showed that the binding energies for most nuclei could be reproduced quite well with a liquid drop model (11). Consequently, the alpha model was revived in at least three different forms.

The simplest of these was formulated in 1937 and is now commonly referred to as the classical $\alpha$-particle (CAP) model. It assumed that all light $\alpha$-nuclei were composed entirely of alpha clusters arranged in a
semi-rigid molecular structure. Wefelmeier (12) is usually given credit for suggesting this model. However, Wheeler (7) independently developed the CAP model for the 1p shell nuclei as groundwork for his more complicated "resonating group structure" technique. Since over half of the original work in this thesis is devoted to the CAP model, we will not elaborate further on the model until Chapter II. The other two forms developed during this period were both α-cluster models and dealt with microscopic calculations of light A=4N nuclei. The first of these, which has already been mentioned, was the "resonating group structure" method introduced by Wheeler (7) in 1937; the other was formulated by Margenau (13) four years later and is now usually referred to as the "generator coordinate" method. Both of these models have been extended and reconsidered in more recent times, and the results of these calculations will be compared with those of the CAP model in Chapter II.

Unfortunately, in 1941 the alpha model suffered a serious setback that hampered further development of the model for over ten years. At that time, Wheeler (14) endeavored to extract a phenomenological α-α potential by analyzing the available data on alpha particle scattering from He⁴ nuclei. After careful analysis, he was forced to conclude that no simple potential could account for the observed cross sections. This meant that the low-lying levels of the ⁸Be resonant state could not be interpreted as the eigenstates of two quasi-bound alpha clusters, and gave good support to the shell-model. Several textbooks have used this argument as direct evidence against the alpha model (15,16). Wheeler's conclusion was actually wrong and was caused by inaccurate data from experiments performed in early 1930. Wheeler politely questioned this possibility in the end of his paper, but
said nothing more. This mistake was not corrected until 1952 when the scattering experiments were repeated with far better resolution.

Comparatively little work was done on the alpha model in the 1950's even after the mistake was corrected. By this time, the independent particle shell model with spin-orbit coupling was so popular that any calculation which did not relate directly to the individual particle states was regarded by many nuclear physicists to be naive and unrealistic. The few papers that were written on the alpha model during this period were mostly elaborations of the three forms noted earlier.

Then in the early 1960's, fast computers became a reality and the two $\alpha$-cluster models that were formulated twenty years earlier were explored in detail. Attempts were also made to solve the three body problem of $^{12}\text{C}$ by assuming the subentities of this nucleus to be three permanent alpha particles. Such a calculation, which has been coined the realistic $\alpha$-particle (RAP) model, yields some interesting results about the effective $\alpha-\alpha$ potential as will be shown in Section IIIG.

The amount of literature on the alpha model written per year has increased considerably during the last five years. This apparent rise in popularity of the alpha model indicates a movement on the part of many nuclear physicists to be more lenient towards a model that was rejected by nearly everyone twenty years earlier. Like other unified models, the alpha model is now viewed by many to be an important modification to the shell model, which may possibly supplement some areas where the shell model is deficient. In addition, the alpha model is not nearly as developed as it should be, and some relatively easy calculations are still possible. The current revival of interest in various forms of alpha models should
therefore persist for five to ten years. By then it will be known whether
this model offers any substantial improvement over other models for light
nuclei.
II. CLASSICAL \( \alpha \)-PARTICLE MODEL

A. Hamiltonian and Basis Functions

As has already been indicated, much of the theory needed for the CAP model is identical to that used in molecular mechanics. A semirigid structure of \( N \) particles has \( 3N \) degrees of freedom. Six of these are needed to characterize the overall rotations and translations of the configuration, and the remaining \( 3N-6 \) coordinates describe various internal vibrations. A rigorous derivation for the Hamiltonian of such a structure is straightforward but long. Standard texts are available on the subject, so only a brief sketch of the procedure will be presented in this work (17,18). It is assumed that the individual particles oscillate quite rapidly compared to their overall collective rotation. One can then separate the classical Hamiltonian into a sum of three parts as

\[
H = H_R + H_V(q, \dot{q}) + H_C.
\]

In this equation, \( H_R \) describes the overall rotations of an effective "rigid" rotor that is formed by keeping the particles fixed in their equilibrium positions. The second term, \( H_V \), describes the internal vibrations of the structure, and is a function of \( 3N-6 \) internal coordinates \( (q) \) and their time derivatives \( (\dot{q}) \) which describe the displacements and velocities of the particles from their equilibrium positions. Usually, one develops this part of the Hamiltonian within the theory of small (harmonic) oscillations, and if this is done, one finds that it is possible to choose these internal coordinates in such a way that \( H_V \) decouples into a sum of \( 3N-6 \) harmonic oscillator terms. These coordinates, which are unique for any structure, are called...
normal coordinates (denoted Q). In general they depend explicitly on the ratios of the force constants between the particles. However, their symmetry properties can be readily obtained from group theory as will be shown in Section C. The last term in Equation 2.1 is the coupling Hamiltonian and contains such terms as the usual Coriolis interaction as well as minor corrections that arise from the harmonic approximation.

One can now quantize the Hamiltonian of Equation 2.1 in the following form

\[ H = H_R + H_V(Q, \dot{Q}) + H_C, \]  

where

\[ H_R = \sum_{\kappa} \frac{L_{\kappa}}{2I_{\kappa}} L_{\kappa}^2 \]  

and

\[ H_V = \sum_{\nu=6}^{\infty} \frac{P_{\nu}^2}{2m_i} + \frac{1}{2} \sum_{\nu} \left( \frac{\lambda_{\nu}^2}{\mu^2} \right) \omega_i Q_{\nu}^2. \]  

In Equation 2.3, \( I_{\kappa} \) is the moment of inertia of the structure with respect to the \( \kappa \)th body-fixed axis, and the \( L_{\kappa} \)'s are the body-fixed angular momentum operators of a rigid rotor. A suitable set of basis functions for diagonalizing the total Hamiltonian in Equation 2.2 can be obtained by setting \( H_C = 0 \). The Hamiltonian is then the sum of rotational and vibrational parts, so the eigenfunctions can be written as

\[ \psi_T = \psi_R \psi_V \equiv \psi_{LM}(\kappa, \beta, \gamma) T_{s1}^{2} H_{\frac{3}{2}}\left(\frac{m_{\omega}}{\mu} Q_{\nu}\right). \]  

The structure is allowed to rotate freely in the laboratory system, so \( L \) and \( M \) must be good quantum numbers of all eigenfunctions. The angles \( \alpha, \beta, \) and \( \gamma \) are the three Euler angles which specify the instantaneous orientation of the body-fixed axes with the space-fixed coordinate system as shown in
Figure 2.1. The quantity \( |\Psi_{LM}(\alpha, \beta, \gamma)|^2 \) then represents the probability of finding the rigid rotor at a particular orientation. In Equation 2.5, \( H_{n_i}(\frac{\mu \omega \gamma}{\hbar}) \) is the \( n_i \)^{th} Hermite function of the \( i \)\textsuperscript{th} normal coordinate.

The Coriolis force for molecules is usually quite small because the frequencies of the normal vibrations are much larger than those of collective rotations, \( (\pi \omega \gg \omega_K) \). In addition, the particles are situated in deep potential wells, so that anharmonic terms in the potential are of minor importance. The energy spectrum of a molecule thus exhibits finely spaced rotational levels on each vibrational eigenstate of the system. \( H_C \) will mix these states somewhat; however, its main contribution comes only from diagonal terms in the matrix Hamiltonian, which systematically reduce the rotational parameters, \( \omega_K \), as the vibrational states increase in energy. This effect is due primarily to repulsive terms in the potential which push the mean positions of the particles outward for excited vibrations.

The Hamiltonian of Equation 2.2 is at best only a rough approximation for the nuclear case. If the CAP model has any validity at all, it is simply because the alpha clusters are correlated long enough to impress some overall molecular structure on the nuclear shell model states. For this reason, no attempt will be made to evaluate \( H_C \) in any quantitative manner for the nuclear structures. However, strong repulsive terms in the potential would be expected to push the mean positions of the particle outward for excited vibrations. We shall therefore qualitatively account for the diagonal contributions of \( H_C \) by allowing the rotational parameters to take on smaller values for excited vibrational states. It should be emphasized that it is possible to obtain good agreement with experiment by using one set of average rotational parameters for all vibrations as has been done in
Figure 2.1. The Euler angles ($\alpha, \beta, \gamma$) are shown which describe the orientation of the body axes ($X', Y', Z'$) relative to the space-fixed coordinate system ($X, Y, Z$). They are defined by the following three passive rotations:

1. a rotation through an angle $\alpha$ about the $Z$ axis,
2. a rotation through an angle $\beta$ about the $Y_1$ axis, and
3. a rotation through an angle $\gamma$ about the $Z'$ axis.
previous papers (19-24). However, by allowing some variation in these parameters, one can obtain better agreement with experiment and also study the variation of the effective rotational parameters with changing normal vibrations.

In order to describe the motions of the rigid rotor, it becomes convenient to define a quantity called the "momental ellipsoid" which is found by plotting the inverse square root of the moment of inertia $\sqrt{\frac{1}{I}}$ along every possible axis of the rotor. The exact shape of the momental ellipsoid depends explicitly on how many of the principal moments of inertia are equal, and separate names are given for each of the three cases (17). When two of the principal moments of inertia are equal, the rotor is called a symmetric top, and the momental ellipsoid has axial symmetry. If all three moments are equal, the momental ellipsoid is a sphere, and the rotor is called a spherical top. If all three moments of inertia are different, the rotor is called an asymmetric top, and the momental ellipsoid has $D_{2h}$ symmetry.

Most of the alpha structures considered in this section will be symmetric rotors with $A_1 = A_2 \neq A_3$. In this case, the Hamiltonian in Equation 2.3 simplifies to

$$H_{\alpha} = A_1 (L_x^2 + L_y^2) + A_3 L_z^2$$

$$= A_1 L_z^2 + L_y^2 (A_3 - A_1).$$

The eigenfunctions for this Hamiltonian are well known in molecular and nuclear physics. Following Rose's notation (25), we define these symmetric top wavefunctions as

$$\Psi_{M, K}^{L} (\alpha, \beta, \gamma) = \sqrt{\frac{8 n^2}{2L+1}} D_{M, K}^{L*} (\alpha, \beta, \gamma).$$
An analytic form for this wavefunction is given in Equations A4 and A5. The quantum number \( L \) denotes the total angular momentum of the state, while \( M \) and \( K \) are the projections of \( L \) on the space-fixed \( z \) axis, and the body-fixed \( z \) axis respectively. The energy levels of the symmetric top are thus simply expressed as

\[
E_R = A_L L (L+1) + \hbar^2 (A_3 - A_L) .
\]  

(2.8)

Besides the usual \((2L+1)\)-fold degeneracy in the \( M \) quantum number, all levels with \( K\neq0 \) are doubly degenerate because the energy depends only on the magnitude of \( K \). (See Figure 2.2b).

For a spherical rotor, all three rotational parameters are equal, and the rotational Hamiltonian of Equation 2.3 becomes

\[
H_R = A_L L^2 .
\]  

(2.9)

The wavefunctions of Equation 2.7 are still eigenfunctions of the Hamiltonian. However, the energy levels for this Hamiltonian are degenerate in both the \( K \) and \( M \) quantum numbers as shown in Figure 2.2a.

Unlike the other two rotors, the wavefunctions for the asymmetric rotor cannot be written in simple form. This can most easily be seen by rewriting Equation 2.3 as

\[
H_R = \left( \frac{A_1 + A_2}{2} \right)(L_x^2 + L_y^2) + A_3 L_z^2 + \left( \frac{A_1 - A_2}{2} \right)(L_x^2 - L_y^2) ,
\]  

(2.10)

or

\[
H_R = \left( \frac{A_1 + A_2}{2} \right)(L_x^2 - L_y^2) + A_3 L_z^2 + \left( \frac{A_1 - A_2}{2} \right)(L_+^2 + L_-^2) .
\]  

(2.11)

In the last equation, the quantities \( L_- \) and \( L_+ \) are raising and lowering operators respectively and are defined as \( L_{\pm} = \pm\frac{1}{i}(L_x \pm iL_y) \) as shown in
Figure 2.2: Energy levels and spins for the three different rotors. Each level is at least $2(2L+1)$-fold degenerate due to the parity and $\hat{M}$ quantum numbers. In the spherical rotor, (a), each level is also $(2L+1)$-fold in the $K$ quantum numbers. For the symmetric rotor, (b), the levels are 2-fold if $K \neq 0$. No additional degeneracy occurs for the asymmetric rotor (c).
Appendix D. The first two terms of Equation 2.11 are diagonal in the symmetric top wavefunction, but the last term connects states with $K$ differing by ±2. The asymmetric top wavefunctions are then

$$\psi_{M}^{L}(\tilde{\tau}, \kappa, B, \gamma) = \sum_{K} a_{M}^{L}(\tilde{\tau}) D_{M}^{L}^{\kappa}(\kappa, B, \gamma).$$

The sum on $K$ is over either even or odd values of $K$, and $N$ is an ordinal number that distinguishes the rotational levels having the same $L$ value. The expansion coefficients, $a_{N}^{L}$, must in general be found by diagonalizing the Hamiltonian of Equation 2.11 among the symmetric top wavefunctions. However, these coefficients are a function of only one parameter which can be defined as

$$\tilde{\eta} = \frac{A_{1}-A_{2}}{2A_{3}-A_{1}-A_{2}}.$$ 

This dependence can most easily be seen by rewriting Equation 2.10 as

$$H_{R} = \frac{(A_{1}+A_{3}+A_{2})}{3} L^{2} + \frac{(2A_{3}-A_{1}-A_{2})}{6} \left[ (2L_{z}^{2} - L_{x}^{2} - L_{y}^{2}) + \frac{3(A_{1}-A_{2})}{(2A_{3}-A_{1}-A_{2})} (L_{x}^{2} - L_{y}^{2}) \right].$$

Any wavefunction that diagonalizes the square braced term in Equation 2.14 also diagonalizes $H$. The wavefunction of this braced term depends only upon the ratio $(A_{1}-A_{2})/(2A_{3}-A_{1}-A_{2})$, while the factor $(2A_{3}-A_{1}-A_{2})/6$ serves as a scale factor for the energy spectrum and $1/3(A_{1}+A_{2}+A_{3})L^{2}$ is merely an additive constant for fixed $L$. This fact will be used later in the calculation of the electron scattering form factors and reduced matrix elements of $^{24}$Mg.

It is important to note that the three rotor Hamiltonians (Equations 2.6, 2.9, and 2.10) have the same symmetry as their corresponding momental
ellipsoids. For example, the symmetric rotor Hamiltonian (Equation 2.6) is invariant under the transformation $(A_1, A_2, A_3) \rightarrow (A_1 \cos \theta + A_2 \sin \theta, -A_1 \sin \theta + A_2 \cos \theta, A_3)$ as well as all other operations of $D_{\infty h}$. Therefore, the wavefunction for the spherical, symmetric, and asymmetric tops generate irreducible representations (IR's) of $O(3)$ (full rotation group), $D_{\infty h}$, and $D_{2h}$ respectively. These symmetries can also be seen in Figure 13 by careful examination of the level degeneracies.

For later use, we state without proof that the symmetry group of the momental ellipsoid for a rigid structure is always a cover group for the structure's spatial point group. This fact will be extremely useful in Section D when it becomes necessary to classify the rotational wavefunctions into IR's of the spatial point group of the structure. Since nearly all of our structures are symmetric tops, the wavefunctions need only be reduced from $D_{\infty h}$ and not from the full rotation group $O(3)$.

B. Bose-Einstein Statistics

Not all of the rotational levels predicted in Figure 2.2 are allowed for a particular $\alpha$-structure. This is because alpha particles are bosons, and Bose-Einstein statistics demand that the only wavefunctions which can occur are those that are invariant under all possible permutations of alpha particles. In order to decide which wavefunctions of Equation 2.5 satisfy this condition, we note that the Hamiltonian in Equation 2.2 is invariant under all group operations which leave the $\alpha$-structure invariant. These operations must be carried out in the body-fixed coordinate system where the mean positions of the alpha clusters are constant in time. Since $H_R$ and $H_V$ also have at least as much symmetry as $H$, each $\Psi_R$ and $\Psi_V$, as well as the
product of $\Psi_R \Psi_V$, must belong to one of the irreducible representations (IR) of the point group. Using Bose-Einstein statistics, one then requires $\Psi_R \Psi_V$ to be symmetric under all operations of the group, and this in turn implies that $\Psi_R$ and $\Psi_V$ must both belong to the same IR. If no normal vibration is excited, both $\Psi_R$ and $\Psi_V$ belong to the completely symmetric IR.

In Table 2.1, the rotational wavefunctions are classified for most of the point groups that will be considered in this work. Standard procedures exist for cataloguing these rotational wavefunctions, and these methods will be described in detail in the next section. The lowest-lying experimental rotation bands of a nucleus are presumably built on the zero-point vibrational mode and must therefore be correlated with the theoretical $K^T$ bands associated with the completely symmetric IR's which are given at the top of each column. With this assumption, one can usually eliminate all but one of the possible structures for each nucleus.

C. Classification of Rotational Wavefunctions

1. Procedure

The wavefunctions $D_{MK}^{L^*}(\alpha)$ are eigenfunctions of the spherical top (Figure 2.2a) and therefore generate IR's of the rotation group $R(3)$ in body coordinates. Since $R(3)$ is a cover group for all rotation point groups, the set of wavefunctions $\left\{ D_{MK}^{L^*}(\alpha,\beta,\gamma), K=-L, \ldots, L \right\}$ forms a $(2L+1)$-fold reducible representation for the point group in question. This reduction must be accomplished so one can find which rotational states are allowed for each IR of the point group (as shown in Table 2.1). Although the reduction procedure has been described in previous papers (26), it will be rederived in the present work using Rose's notation (25) for the rotation matrices.
Table 2.1. Allowed rotational $K^\pi$ bands for each IR (denoted $\Gamma$) of various point groups. Unless otherwise stated, all energy levels with $L=K$ are allowed for each band. Note that parity is conserved within each IR only if the point group includes the inversion operation.

<table>
<thead>
<tr>
<th>$\Gamma$</th>
<th>$K^\pi$ bands</th>
<th>$\Gamma$</th>
<th>$K^\pi$ bands</th>
<th>$\Gamma$</th>
<th>$K^\pi$ bands</th>
<th>$\Gamma$</th>
<th>$K^\pi$ bands</th>
<th>$\Gamma$</th>
<th>$K^\pi$ bands</th>
<th>$\Gamma$</th>
<th>$K^\pi$ bands</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>$0^+ (L \text{ even})$, $2^+$, $4^+$,...</td>
<td>$A_1$</td>
<td>$0^+ (L \text{ odd})$, $2^+$, $4^+$,...</td>
<td>$A_1$</td>
<td>$0^+ (L \text{ even})$, $2^+$, $4^+$,...</td>
<td>$A_1$</td>
<td>$0^+ (L \text{ even})$, $2^+$, $4^+$,...</td>
<td>$A_1$</td>
<td>$0^+ (L \text{ even})$, $2^+$, $4^+$,...</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$B_1$</td>
<td>$0^+ (L \text{ even})$, $2^+$, $4^+$,...</td>
<td>$B_1$</td>
<td>$0^+ (L \text{ even})$, $2^+$, $4^+$,...</td>
<td>$B_1$</td>
<td>$0^+ (L \text{ even})$, $2^+$, $4^+$,...</td>
<td>$B_1$</td>
<td>$0^+ (L \text{ even})$, $2^+$, $4^+$,...</td>
<td>$B_1$</td>
<td>$0^+ (L \text{ even})$, $2^+$, $4^+$,...</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$A_2$</td>
<td>$0^+ (L \text{ odd})$, $2^+$, $4^+$,...</td>
<td>$A_2$</td>
<td>$0^+ (L \text{ odd})$, $2^+$, $4^+$,...</td>
<td>$A_2$</td>
<td>$0^+ (L \text{ odd})$, $2^+$, $4^+$,...</td>
<td>$A_2$</td>
<td>$0^+ (L \text{ odd})$, $2^+$, $4^+$,...</td>
<td>$A_2$</td>
<td>$0^+ (L \text{ odd})$, $2^+$, $4^+$,...</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$B_2$</td>
<td>$0^+ (L \text{ odd})$, $2^+$, $4^+$,...</td>
<td>$B_2$</td>
<td>$0^+ (L \text{ odd})$, $2^+$, $4^+$,...</td>
<td>$B_2$</td>
<td>$0^+ (L \text{ odd})$, $2^+$, $4^+$,...</td>
<td>$B_2$</td>
<td>$0^+ (L \text{ odd})$, $2^+$, $4^+$,...</td>
<td>$B_2$</td>
<td>$0^+ (L \text{ odd})$, $2^+$, $4^+$,...</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$E$</td>
<td>$1^+$, $3^+$, $5^+$,...</td>
<td>$E_g$</td>
<td>$1^+$, $3^+$, $5^+$,...</td>
<td>$E_e$</td>
<td>$1^+$, $3^+$, $5^+$,...</td>
<td>$E_e$</td>
<td>$1^+$, $3^+$, $5^+$,...</td>
<td>$E_e$</td>
<td>$1^+$, $3^+$, $5^+$,...</td>
<td>$E_e$</td>
<td>$1^+$, $3^+$, $5^+$,...</td>
</tr>
<tr>
<td>$E_u$</td>
<td>$1^+$, $3^+$, $5^+$,...</td>
<td>$E_u$</td>
<td>$1^+$, $3^+$, $5^+$,...</td>
<td>$E_u$</td>
<td>$1^+$, $3^+$, $5^+$,...</td>
<td>$E_u$</td>
<td>$1^+$, $3^+$, $5^+$,...</td>
<td>$E_u$</td>
<td>$1^+$, $3^+$, $5^+$,...</td>
<td>$E_u$</td>
<td>$1^+$, $3^+$, $5^+$,...</td>
</tr>
<tr>
<td>$E_3$</td>
<td>$1^+$, $3^+$, $5^+$,...</td>
<td>$E_3$</td>
<td>$1^+$, $3^+$, $5^+$,...</td>
<td>$E_3$</td>
<td>$1^+$, $3^+$, $5^+$,...</td>
<td>$E_3$</td>
<td>$1^+$, $3^+$, $5^+$,...</td>
<td>$E_3$</td>
<td>$1^+$, $3^+$, $5^+$,...</td>
<td>$E_3$</td>
<td>$1^+$, $3^+$, $5^+$,...</td>
</tr>
</tbody>
</table>
2. **Symmetric and asymmetric rotors**

Only two types of rotations need to be considered for structures that are not spherical rotors. These are:

1. \(C_n\) — an \(n\)-fold rotation about the body-fixed \(z\) axis, and
2. \(C_{2p}\) — a 2-fold rotation about the \(p^{th}\) axis in the \(xy\) plane.

Since \(C_n\) implies a rotation about the \(z\) axis through an angle \(\alpha = \frac{2\pi}{n}\), we find from Equation B6 that

\[
C_n \, D_{mK}^{L^*}(\alpha) = e^{i \frac{2\pi}{n} K} D_{mK}^{L^*}(\alpha) .
\]

(2.15)

All of the structures in the present work will have at least two 2-fold axes in the \(xy\) plane. If the \(p^{th}\) 2-fold axis subtends an angle \(\beta\) with the \(x\) axis, one gets from Equation B7

\[
C_2^p \, D_{mK}^{L^*}(\alpha) = C_2^{xy}(\beta) D_{mK}^{L^*}(\alpha) = e^{i \frac{2\pi}{n} K^p} D_{m, K - K}^{L^*}(\alpha) .
\]

(2.16)

Besides \(L\) and \(M\), parity is also a good quantum number of any rotational state. Therefore one must consider basis states of the full rotational group \(O(3)\) which includes rotations and reflections. This can be easily accomplished in a formal, mathematical procedure by introducing a parity quantum number (denoted \(\Pi\)) to the basis functions and stating that the inversion operator \((I)\) operates on the states in the following way

\[
I \, D_{mK}^{L \Pi^*}(\alpha, \xi) = D_{mK}^{L \Pi^*}(\alpha, \xi \xi) = \pm D_{mK}^{L \Pi^*}(\alpha, \xi) .
\]

(2.17)

Note that the parameter space has doubled; \(\xi\) represents either the identity or inversion element. For convenience, the latter variable will be suppressed in all subsequent rotational wavefunctions that include the parity quantum number, so we simply write
where $\alpha$ now characterizes the parameter space of the full rotational group, $SO(3)$. The physical concept of parity on a non-planar molecular structure is more complicated and is explained by assuming that these structures have a certain probability for tunneling through a potential barrier which allows the system to go from a right-handed to a left-handed coordinate system \(^{19,20,27}\). The exact tunneling procedure depends on the shape of the configuration and will be considered in detail for the $\alpha$-structure of \(^{20}\)Ne in Section H. Parity, however, can be easily understood for planar or linear structures, since the inversion of all particles is then equivalent to an appropriate 2-fold rotation as will be shown later in Section G for the $\alpha$-structures of \(^{8}\)Be and \(^{12}\)C. Several authors have specifically worried about the parity assignments of wavefunctions, not only in the CAP model \(^{21}\), but also for the collective rotor \(^{28}\) and SU\(_{\frac{3}{2}}\) \(^{29}\) models. Consequently, whenever possible we will note the equivalence of parity assignments found by physically inverting the $\alpha$-structure to those obtained from the mathematical formalism of the present section.

All operations of $SO(3)$ can be represented either as a rotation or as a rotation multiplied by the inversion element. In this way, one can easily show how reflections must operate on the wavefunctions. The ones that need to be considered for symmetric or asymmetric tops are:

1. $S_n$—an $n$-fold rotation about the $z$ axis followed by a reflection in the $xy$ plane (denoted $\sigma'_{xy}$), and

2. $\sigma'_{p}$—a reflection in a vertical plane, ($p$ is a running label that distinguishes different planes).
It can be easily shown that \( S_{xy} I = \sigma_{xy} C_2 \), which implies that \( \sigma_{xy} = IC_2 \). Therefore, the operation \( S_n \) is actually \( S_n = \sigma_{xy} C_2 = IC_2 C_n \). From Equations 2.15 and 2.17, we then obtain

\[
S_n D_{m,n}^{L,\pi^*}(\eta) = \pm e^{i \pi \kappa \left( \frac{\pi}{2} + \frac{\eta}{2} \right)} D_{m,n}^{L,\pi^*}(\eta).
\] (2.19)

In a similar fashion, if one considers \( \sigma_v^p \) to be a reflection in a vertical plane with the plane subtending an angle \( \beta \) with the x axis, it can be shown that

\[
\sigma_v^p \equiv \sigma_v(\beta) = I C_2^{xy} \left( \frac{\pi}{2} + \beta \right),
\]

and from Equations 2.16 and 2.17, one finds

\[
\sigma_v^p D_{m,n}^{L,\pi^*}(\eta) = \pm (-)^L e^{-2 \pi \kappa \left( \frac{\pi}{2} + \beta \right)} D_{m,n}^{L,\pi^*}(\eta).
\] (2.20)

It is important to note that the operations mentioned so far do not mix wavefunctions with different values of \( |k| \). The necessary reduction can then proceed from IR's of \( D_6 \) instead of \( O(3) \). Using the notation

\[
|L^\pi M K\rangle \equiv \sqrt{\frac{2L+1}{8\pi^2}} D_{m,n}^{L,\pi^*}(\eta),
\] (2.21)

one finds a suitable choice of basis states to be \( |L^\pi M 0\rangle \) and \( |L^\pi M K\rangle \) for \( K=0 \) and \( K>0 \) respectively. Using these basis states, along with Equations 2.15, 2.16, 2.19 and 2.20, one can find the matrix representatives of the necessary operations in a straightforward manner. For \( K=0 \), one finds

\[
D^{\sigma_v^p}(C_n) = 1, \quad D^{\sigma_v^p}(C_2^p) = (-)^L
\]

\[
D^{\sigma_v^p}(S_n) = \pm 1, \quad D^{\sigma_v^p}(\sigma_v^p) = \pm (-)^L.
\] (2.22)
and for $K\neq 0$,

$$D^{K,\pi}_n(C_n) = \begin{pmatrix} e^{i\frac{2\pi K}{n}} & 0 \\ 0 & e^{-i\frac{2\pi K}{n}} \end{pmatrix} \quad D^{K,\pi}_n(C_2^p) = (-)^L \begin{pmatrix} 1 & e^{2iK\beta} \\ e^{2iK\beta} & 1 \end{pmatrix}$$

$$D^{K,\pi}_n(s_n) = \begin{pmatrix} e^{i\pi K(1+\frac{2}{n})} & 0 \\ 0 & e^{-i\pi K(1+\frac{2}{n})} \end{pmatrix} \quad D^{K,\pi}_n(\sigma^p_v) = \pm (-)^L \begin{pmatrix} 1 & e^{2iK(1+\beta)} \\ e^{2iK(1+\beta)} & 1 \end{pmatrix}$$  (2.23)

In order to find what IR of the point group each IR of $D_{\omega h}$ reduces to, one needs only find the trace of these matrices which are

$$\chi^{0,\pi}_n(C_n) = 1 \quad \chi^{0,\pi}_n(C_2^p) = (-)^L$$

$$\chi^{0,\pi}_n(s_n) = \pm \quad \chi^{0,\pi}_n(\sigma^p_v) = \pm (-)^L$$  (2.24)

for $K=0$, and

$$\chi^{K,\pi}_n(C_n) = 2\cos\left(\frac{2\pi K}{n}\right) \quad \chi^{K,\pi}_n(C_2^p) = 0$$

$$\chi^{K,\pi}_n(s_n) = \pm 2\cos\left((1+\frac{2}{n})\pi K\right) \quad \chi^{K,\pi}_n(\sigma^p_v) = 0$$  (2.25)

for $K\neq 0$. It is very interesting to note that the traces of $C_2^p$ and $\sigma^p_v$ are independent of $\beta$. Such a fact indicates that the reduction process is independent of the exact direction of the x axis in the equatorial (xy) plane of the configuration.

We shall now carry out the reduction for one particular subgroup of $D_{\omega h}$. Figure 2.3 shows a configuration of five particles exhibiting $D_{2d}$ symmetry. (It will be shown in Section H that this structure is the appropriate one for $^{20}$Ne.) The character table, showing the five IR's and symmetry classes of $D_{2d}$, is given in Table 2.2. Then in Table 2.3, we make use of Equations 2.24 and 2.25 to find the characters of the IR's of $D_{\omega h}$ under the
A D$_{2d}$ structure is invariant under three 2-fold rotations (C$_{2}^{x}$, C$_{2}^{y}$, and C$_{2}^{z}$) and two reflections (σ$_{d}^{\prime}$ and σ$_{d}^{\prime\prime}$) as shown above. The structure is also invariant under two S$_{4}$ operations which involve a rotation of 90° along the z axis followed by a reflection in the xy plane.

Table 2.2. Character table for D$_{2d}$.

<table>
<thead>
<tr>
<th></th>
<th>D$_{2d}$</th>
<th>E</th>
<th>C$_{2}$</th>
<th>2S$_{4}$</th>
<th>2C$_{2}^{\prime}$</th>
<th>2σ$_{d}^{\prime}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A$_{1}$</td>
<td></td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>A$_{2}$</td>
<td></td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>B$_{1}$</td>
<td></td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>B$_{2}$</td>
<td></td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
</tr>
<tr>
<td>E</td>
<td></td>
<td>2</td>
<td>-2</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
Table 2.3. Table showing the reduction of rotational basis functions for $D_{2d} \cong D_{2h}$.

<table>
<thead>
<tr>
<th>$L^\pi K$</th>
<th>$E$</th>
<th>$C_2$</th>
<th>$2S_4$</th>
<th>$2C_2'$</th>
<th>$2\sigma_d'$</th>
<th>IR's of $D_{2d}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L^+0$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$A_1$ (L even); $A_2$ (L odd)</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>$(-)^L$</td>
<td>$(-)^L$</td>
<td>E</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>-2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>$B_{1}+B_{2}$</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>-2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>E</td>
</tr>
<tr>
<td>4</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>$A_1+A_2$</td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td>-2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>E</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>2</td>
<td>-2</td>
<td>0</td>
<td>0</td>
<td>$B_{1}+B_{2}$</td>
</tr>
<tr>
<td>$L^-0$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$B_1$ (L even); $B_2$ (L odd)</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>$(-)^L$</td>
<td>$(-)^L$</td>
<td>E</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>-2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>$A_1+A_2$</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>-2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>E</td>
</tr>
<tr>
<td>4</td>
<td>2</td>
<td>2</td>
<td>-2</td>
<td>0</td>
<td>0</td>
<td>$B_1+B_2$</td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td>-2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>E</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>$A_1+A_2$</td>
</tr>
</tbody>
</table>
$D_{2d}$ operations. The standard formulas needed for performing the necessary reduction are (30, p. 107)

$$\chi^\rho(R) = \sum_\lambda A_\rho^\lambda \chi^\lambda(R)$$

(2.26)

and

$$A_\rho^\lambda = \frac{1}{n_c} \sum_\text{c} n_\text{c} \chi^\rho(\text{c}) \chi^\lambda(\text{c})$$

(2.27)

The quantity $\chi^\rho(R)$ is the trace of the matrix representation $D^\rho(R)$ for the reducible representation of $R$, and $\chi^\lambda(R)$ is the character for the corresponding IR of $D_{2d}$ labeled by $\lambda$. Also, $A_\rho^\lambda$ specifies the number of times each IR is contained in the reducible representation. In Equation 2.27, the sum is over classes of operations, and $n_c$ denotes the number of operations included in each class. The results of such a calculation are shown in the last column of Table 2.3. From this table, we can now extract the spins and parities of wavefunctions allowed for each IR of $D_{2d}$ as is shown in Table 2.4. The allowed wavefunctions can be tabulated more efficiently by noting only the $K^\text{th}$ bands as was done in Table 2.1. Since the procedure for reducing the $D_{2h}$ IR's to other finite subgroups is the same as that of $D_{2d}$, we merely quote the results (Table 2.1) for all other symmetric top point groups that will be considered in Section H.

3. Spherical rotors

Only four spatial point groups exist which are not subgroups of $D_{2h}$. Two of these are invariant under the rotations of a tetrahedron ($T_d$ and $T_h$), and the other two have octahedral ($O_h$) and icosahedral ($I_h$) symmetry respectively. The reduction of rotational basis functions for these point groups must proceed from IR's of the full rotation group $O(3)$. In finding the
Table 2.4. The quantum numbers for the allowed rotational wavefunctions (denoted $L_{JK}$) are listed for each IR of $D_{2d}$.

<table>
<thead>
<tr>
<th>0$^+$</th>
<th>0$^-$</th>
<th>1$^+$</th>
<th>1$^-$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2$^+_0$</td>
<td>2$^-_0$</td>
<td>2$^+_0$</td>
<td>2$^-_0$</td>
</tr>
<tr>
<td>4$^+_0$</td>
<td>4$^-_0$</td>
<td>4$^+_0$</td>
<td>4$^-_0$</td>
</tr>
<tr>
<td>6$^+_0$</td>
<td>6$^-_0$</td>
<td>6$^+_0$</td>
<td>6$^-_0$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>A$_1$</th>
<th>B$_1$</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>0$^-$</td>
<td>0$^-$</td>
<td>1$^+$</td>
</tr>
<tr>
<td>3$^+_2$</td>
<td>3$^-_2$</td>
<td>1$^-$</td>
</tr>
<tr>
<td>5$^+_4$</td>
<td>5$^-_4$</td>
<td>2$^+$</td>
</tr>
<tr>
<td>6$^+_6$</td>
<td>6$^-_6$</td>
<td>2$^-$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>1$^+$</th>
<th>1$^-$</th>
<th>2$^+$</th>
<th>2$^-$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0$^-$</td>
<td>0$^-$</td>
<td>2$^+_2$</td>
<td>2$^-_2$</td>
</tr>
<tr>
<td>3$^+_2$</td>
<td>3$^-_2$</td>
<td>4$^+_2$</td>
<td>4$^-_2$</td>
</tr>
<tr>
<td>5$^+_2$</td>
<td>5$^-_2$</td>
<td>5$^+_4$</td>
<td>5$^-_4$</td>
</tr>
<tr>
<td>6$^+_6$</td>
<td>6$^-_6$</td>
<td>6$^+_6$</td>
<td>6$^-_6$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>A$_2$</th>
<th>B$_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1$^-$</td>
<td>0$^-$</td>
</tr>
<tr>
<td>3$^+_2$</td>
<td>3$^-_2$</td>
</tr>
<tr>
<td>5$^+_4$</td>
<td>5$^-_4$</td>
</tr>
<tr>
<td>6$^+_6$</td>
<td>6$^-_6$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>1$^+$</th>
<th>1$^-$</th>
<th>2$^+$</th>
<th>2$^-$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0$^-$</td>
<td>0$^-$</td>
<td>2$^+_2$</td>
<td>2$^-_2$</td>
</tr>
<tr>
<td>3$^+_2$</td>
<td>3$^-_2$</td>
<td>4$^+_2$</td>
<td>4$^-_2$</td>
</tr>
<tr>
<td>5$^+_2$</td>
<td>5$^-_2$</td>
<td>5$^+_4$</td>
<td>5$^-_4$</td>
</tr>
<tr>
<td>6$^+_6$</td>
<td>6$^-_6$</td>
<td>6$^+_6$</td>
<td>6$^-_6$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>1$^+$</td>
</tr>
<tr>
<td>3$^+_3$</td>
</tr>
<tr>
<td>4$^+_3$</td>
</tr>
<tr>
<td>5$^+_5$</td>
</tr>
<tr>
<td>6$^+_5$</td>
</tr>
</tbody>
</table>
characters of the various IR's for each rotation, we do not have to consider the axis direction. This differs from the symmetric rotor where it was found that a 2-fold rotation about the z axis generated different characters than the same rotation about an axis in the xy plane. Thus, the only rotation that need be considered for the present case is a rotation by an angle $\alpha$ about any axis. The character of such an operation can be readily evaluated by performing the rotation about the z axis. Choosing the basis functions as

$$ | L \pi, M, L \rangle $$

$$ | L \pi, M, L-1 \rangle $$

$$ \vdots $$

$$ | L \pi, M, -L \rangle $$

one can show that the corresponding matrix representation is

$$ D^{L, \pi}(C\omega) = \begin{pmatrix}
  e^{iL\alpha} & 0 & \cdots & 0 \\
  0 & e^{i(l-1)\alpha} & \cdots & 0 \\
  \vdots & \vdots & \ddots & \vdots \\
  0 & 0 & \cdots & e^{-iL\alpha}
\end{pmatrix} \quad (2.28) $$

The trace of this matrix can be shown to be (30, p. 336)

$$ \chi^{L, \pi}(C\omega) = \sum_{k=-L}^{L} e^{iM\alpha} = \frac{\sin \left( \frac{L+\frac{1}{2})\pi}{2} \right)}{\sin \frac{\pi}{2}} \quad (2.29) $$

Remembering that $C_n$ denotes a rotation by an angle $\alpha = \frac{2\pi}{n}$, we obtain

$$ \chi^{L, \pi}(C_n) = \frac{\sin \left( \frac{L+\frac{1}{2})\pi}{n} \right)}{\sin \frac{\pi}{n}} \quad (2.30) $$

The only other operation that need be considered is $S_n$, an n-fold rotation followed by a reflection in the plane perpendicular to the axis of rotation.
From Equation 2.18, we know that 5\(^n\) = 1020\(^n\), so
\[
X^{L, \pi}(5^n) = \pm \frac{\sin \left\{ (\frac{L+\frac{1}{2}}{2}) \pi (i+\frac{\pi}{n}) \right\}}{\sin \left\{ \frac{\pi}{2} (i+\frac{\pi}{n}) \right\}}.
\]  
(2.31)

It should be noted that \(S_1\) and \(S_2\) correspond to a reflection through a plane \((\sigma)\) and inversion \((I)\) respectively.

Again, we shall carry out the procedure for one particular subgroup of \(O(3)\). In Chapter IV, we shall be particularly interested in the tetrahedral \((T_d)\) group, so this point group will be the one considered. Figure 2.4 shows four particles located at the corners of a tetrahedron (as is supposed to be the case for \(^{16}O\)), and the character table for \(T_d\) is given in Table 2.5. Using the Equations 2.29 and 2.30, one can again find the necessary characters for the classes of \(T_d\) as shown in Table 2.6. Using the results of this table, we can then obtain the spins and parities allowed for each \(IR\) (Table 2.7). Notice that \(K^p\) bands are no longer distinguishable as they were for symmetric tops.

D. Normal Vibrations

If the vibrational part of the Hamiltonian is to remain invariant under the operations of the point group, the following conditions must be met:

1. A nondegenerate normal mode will be either symmetrical or antisymmetrical with respect to each operation of the point group of the undistorted configuration.

2. Each symmetry operation of the group will transform a member of a degenerate set of vibrations into linear combinations of the members of this degenerate set.
Figure 2.4. Tetrahedral structure of four particles.

Table 2.5. Character table for the $T_d$ point group

<table>
<thead>
<tr>
<th>$T_d$</th>
<th>$E$</th>
<th>$8C_3$</th>
<th>$3C_2$</th>
<th>$6\sigma_d$</th>
<th>$6S_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$A_2$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>$E$</td>
<td>2</td>
<td>-1</td>
<td>2</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$T_1$</td>
<td>3</td>
<td>0</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
</tr>
<tr>
<td>$T_2$</td>
<td>3</td>
<td>0</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
</tr>
</tbody>
</table>
Table 2.6. Reduction of the $O(3)$ IR's with respect to the $T_d$ point group.

<table>
<thead>
<tr>
<th>$L^\pi$</th>
<th>E</th>
<th>$8C_3$</th>
<th>$3C_2$</th>
<th>$6\sigma_d$</th>
<th>$6S_4$</th>
<th>IR's of $T_d$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0$^+$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>$A_1$</td>
</tr>
<tr>
<td>1$^+$</td>
<td>3</td>
<td>0</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>$T_1$</td>
</tr>
<tr>
<td>2$^+$</td>
<td>5</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>$E+T_2$</td>
</tr>
<tr>
<td>3$^+$</td>
<td>7</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>$A_2^+T_1+T_2$</td>
</tr>
<tr>
<td>4$^+$</td>
<td>9</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>$A_1^+E+T_1+T_2$</td>
</tr>
<tr>
<td>5$^+$</td>
<td>11</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>$E+2T_1+T_2$</td>
</tr>
<tr>
<td>6$^+$</td>
<td>13</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>$A_1^+A_2^+E+T_1+2T_2$</td>
</tr>
<tr>
<td>7$^+$</td>
<td>15</td>
<td>0</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>$A_2^+E+2T_1+2T_2$</td>
</tr>
<tr>
<td>8$^+$</td>
<td>17</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>$A_2^+2E+2T_1+2T_2$</td>
</tr>
<tr>
<td>0$^-$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>$A_2$</td>
</tr>
<tr>
<td>1$^-$</td>
<td>3</td>
<td>0</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>$T_2$</td>
</tr>
<tr>
<td>2$^-$</td>
<td>5</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>$E+T_1$</td>
</tr>
<tr>
<td>3$^-$</td>
<td>7</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>$A_1^+T_1+T_2$</td>
</tr>
<tr>
<td>4$^-$</td>
<td>9</td>
<td>0</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>$A_2^+E+T_1+T_2$</td>
</tr>
<tr>
<td>5$^-$</td>
<td>11</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>$E+T_1+2T_2$</td>
</tr>
<tr>
<td>6$^-$</td>
<td>13</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>$A_1^+A_2^+E+2T_1+T_2$</td>
</tr>
<tr>
<td>7$^-$</td>
<td>15</td>
<td>0</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>$A_1^++E+2T_1+2T_2$</td>
</tr>
<tr>
<td>8$^-$</td>
<td>17</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>$A_2^+2E+2T_1+2T_2$</td>
</tr>
</tbody>
</table>
Table 2.7. Table showing the number of times each IR of the T_d point group contains a rotational wavefunction of spin and parity L^+.

<table>
<thead>
<tr>
<th></th>
<th>0^+</th>
<th>1^+</th>
<th>2^+</th>
<th>3^+</th>
<th>4^+</th>
<th>5^+</th>
<th>6^+</th>
<th>7^+</th>
<th>8^+</th>
<th>1^-</th>
<th>2^-</th>
<th>3^-</th>
<th>4^-</th>
<th>5^-</th>
<th>6^-</th>
<th>7^-</th>
<th>8^-</th>
<th>9^-</th>
</tr>
</thead>
<tbody>
<tr>
<td>\Lambda_1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>\Lambda_2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
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<td>1</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>\Gamma_1</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>\Gamma_2</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>2</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>\Gamma_3</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>\Gamma_4</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>2</td>
<td></td>
</tr>
</tbody>
</table>

34b
In order for these requirements to hold, the normal modes must belong to an IR of the point group.

In the present work, we need only show how many normal coordinates belong to each IR of the group. This is most easily accomplished by finding the reducible representation generated by the 3N degrees of freedom, and then resolving this representation into its IR components. The rotation and translation coordinates belong to definite IR's, so they can be removed after the reduction.

The exact procedure for finding these modes can be best explained by considering a specific example. Figure 2.5 shows the same \( D_{2d} \) configuration of five particles considered in the previous section. Also shown are the fifteen internal cartesian coordinates which are appropriate for finding \( \chi^p(R) \). These traces can readily be found by summing the diagonal contributions of \( \rho^p(R) \) (as exemplified in Table 2.8). By applying Equation 2.27 to the reducible representation, one can then resolve the representation into its IR components (Table 2.8). The above method for classifying normal modes will be used many times throughout the thesis for different \( \alpha \)-structures. Since the method is the same in all cases, we shall only tabulate the results.

As has already been noted, the spatial symmetry of a structure cannot usually determine the exact shape of a normal mode. This will occur only if an IR contains one normal vibration. If two or more normal modes belong to the same IR, one must be satisfied with constructing orthogonal "symmetry coordinates" which transform under the conditions imposed by the IR. The normal modes for the IR will then be linear combinations of these symmetry coordinates, the coefficients of which depend on the force constants between
Figure 2.5. A $D_{2d}$ configuration of five particles and its fifteen degrees of freedom.

Table 2.8. Characters for the IR's of $D_{2d}$ and also the reducible representation $\rho$ which is generated by the fifteen internal coordinates of Figure 2.5. Also shown is the tensor sum of $\rho$ into its IR's. The bracketed IR's must be subtracted since they represent the six translations and rotations.

<table>
<thead>
<tr>
<th></th>
<th>$E$</th>
<th>$C_2^z$</th>
<th>$2S_A$</th>
<th>$2C_2^1$</th>
<th>$2\sigma_d$</th>
<th>Translations, Rotations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>$R_z$</td>
</tr>
<tr>
<td>$A_2$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td></td>
</tr>
<tr>
<td>$B_1$</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>$T_z$</td>
</tr>
<tr>
<td>$B_2$</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>$(T_x, T_y); (R_x, R_y)$</td>
</tr>
<tr>
<td>$E$</td>
<td>2</td>
<td>-2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>$\rho$</td>
<td>15</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

$\rho = A_1 + A_1 + B_1 + B_2 + E + E + [A_2 + B_2 + E + E]$
particles. The symmetry coordinates can usually be found by inspection, but they can also be calculated in a straightforward manner using the "projection operator" technique (30, p. 113). Figure 2.6 shows the nine symmetry coordinates for the $D_{2d}$ structure considered earlier. The only coordinate that is a genuine normal mode is the twisting vibration of $B_1$ symmetry. These symmetry coordinates are never used explicitly in the present work, so they will not be displayed for any of the other structures.

E. Electron Scattering Form Factors

The charge distribution of the nucleus for the CAP model is given by

$$\rho (x, \vec{r}_i) = \frac{2}{\pi} \sum_{i=1}^{n} \rho_0 (|x - \vec{r}_i|) \quad ,$$

(2.32)

where $\rho_0 (r)$ is the spherical charge density of each alpha particle normalized to unity, $n$ is the number of alpha clusters, and $\vec{r}_i$ is the position of the $i^{th}$ alpha particle. Using this distribution and the Born approximation, one can derive a formula for the differential electron scattering cross section in a long, but straightforward manner. The procedure is well known, since several authors have used the method for predicting the form factors for various $\alpha$-structures (31-36). However, as far as I am aware, only a brief sketch of the derivation has been published (34), so a formal derivation of the theoretical form factors should be included in the present work.

The Hamiltonian that one needs to consider is

$$H = H_n + H_e + H' \quad ,$$

(2.33)

where $H_n$ and $H_e$ are the Hamiltonians for the nucleus and free electron respectively, and $H'$ is the perturbing potential which has the form

$$H' = \int d^3 r' \rho_n (r') \frac{e^2}{|x - x'|} \quad .$$

(2.34)
Figure 2.6. Possible symmetry modes for the $D_{2d}$ structure of $^{20}\text{Ne}$. The only genuine normal vibration is the $B_1$ twisting mode.
In the last equation, the integration is carried out over the laboratory coordinates, and $r$ is the position of the electron. The charge density of the nucleus naturally depends on the nuclear wavefunctions and is normalized to the nuclear charge, $Ze$.

Hofstadter has shown (37) that the differential cross section in the Born approximation between initial and final states with spins $I$ and $I'$ is

$$
\left( \frac{d\sigma}{d\Omega} \right)_{\text{point}} = \left| F_{II'} \right|^2.
$$

(2.35)

The first factor is the Mott-scattering cross section for electrons

$$
\left( \frac{d\sigma}{d\Omega} \right)_{\text{point}} = \left( \frac{2 \mu^2}{E_0} \right) \frac{\cos^2 \frac{\Theta}{2}}{\sin^2 \frac{\Theta}{2}} \frac{1}{1 + \left( \frac{2E_0}{M^2c^4} \right) \sin^2 \frac{\Theta}{2}},
$$

(2.36)

where $\Theta$ is the scattering angle, $E_0$ is the incident energy of the electron, and $M$ is the mass of the target nucleus. The last term can be expressed as

$$
\left| F_{II'} \right|^2 = \frac{|<\Phi|H'|\Phi>|^2}{|<\Phi|H'|\Phi>|^2_{\text{point}}}. \quad (2.37)
$$

We shall therefore be interested in two types of matrix elements of Equation 2.37. The first solution considers the nucleus as a point, and the wavefunctions will simply be those of a free electron

$$
|\tilde{\Phi}> \equiv u_f e^{i \frac{q'}{2L}} / L^{\frac{3}{2}}
$$

$$
|\phi> \equiv u_i e^{i \frac{q}{2L}} / L^{\frac{3}{2}}, \quad (2.38)
$$

where $u_i$ and $u_f$ are the four component spinors common to solutions of the Dirac equation, and $q$ and $q'$ are the momenta of the incoming and scattered electron respectively. The second matrix element we want to calculate includes the CAP model wavefunctions. For the present, we shall be concerned only with transitions among states belonging to the ground state rotational
band. The vibrational modes of Equation 2.5 do not then have to be considered, and the initial and final states of Equation 2.37 can be expressed as

\[ |i'\rangle = \mathcal{Q}_{L'M'}(\alpha) U_e e^{i \frac{q_i' \cdot \alpha}{L}} \]

\[ |f\rangle = \mathcal{Q}_{L'M'}(\alpha) U_f e^{i \frac{q_f' \cdot \alpha}{L}} . \]  

(2.39)

In evaluating the terms of Equation 2.37, one does not have to consider the 4-component spinors \(\psi_i\) or \(\psi_f\) since they will contribute the same multiplicative factor in both the numerator and denominator (37). Defining the momentum transfer as \(q = q' - q\), and \(Z\) as the number of proton charges in the nucleus, one can evaluate the matrix element of the point nucleus using Equations 2.34 and 2.38 as follows:

\[ \langle f' | H' | i' \rangle_{\text{point}} = \int d^3r e^{i \frac{(q' - q) \cdot \alpha}{L}} \int \frac{d^3r' Z e^{2}}{\left| x - x' \right|} \mathcal{S}(\alpha') \]

\[ = \frac{Z e^{2}}{L^3} \int \frac{d^3r e^{i \frac{Q \cdot \alpha}{\alpha^2}}}{\alpha} \left( \frac{q' - q}{\alpha} \right) \int_{0}^{\infty} \sin(q \varrho) \mathcal{A}(q \varrho) . \]

(2.40)

The last integral is indeterminant, but can be evaluated if one allows for the screening of the atomic electrons. Correcting for this effect, the interaction potential becomes \(\frac{Ze^{2}}{\left| x - x' \right|} \exp(-\frac{1}{a \left| x - x' \right|})\), where \(a\) is a distance of atomic dimensions (38, p. 274). The last integral would then be

\[ \int_{0}^{\infty} \sin(q \varrho) e^{-\frac{(r \varrho)}{a \varrho}} \mathcal{A}(q \varrho) = \frac{1}{1 + \frac{1}{a^2 q^2}} \approx 1 , \]

and the denominator of Equation 2.37 therefore has the value

\[ \left| \langle f' | H' | i' \rangle \right|^2_{\text{point}} = \frac{16 \pi^2 Z^2 e^4}{L^6 Q^2} . \]

(2.41)

The integral involving CAP model wavefunctions is far more complicated.
From Equations 2.32 and 2.34 one has

\[ \langle \Psi | \hat{H} \hat{H} | \Psi \rangle = \sum_{i=1}^{n} \int \frac{d^3 \Psi_{i}^* \Psi_{i} \int \frac{d^3 \Psi^* \Psi \int \frac{d^3 \rho}{\pi^2 \rho^2} \int \frac{d^3 \rho_1}{\pi^2 \rho_1^2} \int \frac{d^3 \rho_2}{\pi^2 \rho_2^2} \frac{\rho_0(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)}{\mathbf{x}_1 - \mathbf{x}_2} \mathbf{Q} \cdot \mathbf{R} \rangle \]

The last integral can be evaluated by letting \( r_i = r_i' - r_i \).

\[ \int d^3 r \left[ \cdots \right] = \sum_{i=1}^{n} \int d^3 r_i \int \frac{d^3 \rho}{\pi^2 \rho^2} \frac{\rho_0(r_i)}{\mathbf{x}_1 + \mathbf{r}_i - \mathbf{x}_3} \]

\[ = \sum_{i=1}^{n} \int d^3 r_i \int \frac{d^3 \rho}{\pi^2 \rho^2} \frac{\rho_0(r_i)}{\mathbf{Q} \cdot \mathbf{R} + \mathbf{R} - \mathbf{x}_3} \]

\[ = \frac{2 \pi}{\rho} \sum_{i=1}^{n} \int \frac{d^3 \rho}{\pi^2 \rho^2} \int \frac{d^3 \rho_1}{\pi^2 \rho_1^2} \int \frac{d^3 \rho_2}{\pi^2 \rho_2^2} e^{i \mathbf{Q} \cdot (\mathbf{R}_1 - \mathbf{r}_1)} f_0(\rho) \]

In the last equation, we have assumed all alpha particles have the same charge distribution so that \( f_0(\rho) \), the Fourier transform of \( \rho_0(r) \), is independent of the particle label. The last two integrals of Equation 2.43 are then

\[ \int d^3 r \left[ \cdots \right] = \frac{2 \pi}{\rho} \sum_{i=1}^{n} \int \frac{d^3 \rho}{\pi^2 \rho^2} f_0(\rho) \int \frac{d^3 \rho_1}{\pi^2 \rho_1^2} \int \frac{d^3 \rho_2}{\pi^2 \rho_2^2} e^{i \mathbf{Q} \cdot (\mathbf{R}_1 - \mathbf{r}_1)} \]

Substituting this quantity into Equation 2.43 we find

\[ \langle \Psi | \hat{H} \hat{H} | \Psi \rangle = \frac{2 \pi}{\rho} \sum_{i=1}^{n} \int \frac{d^3 \rho}{\pi^2 \rho^2} f_0(\rho) \int \frac{d^3 \rho_1}{\pi^2 \rho_1^2} \int \frac{d^3 \rho_2}{\pi^2 \rho_2^2} e^{i \mathbf{Q} \cdot (\mathbf{R}_1 - \mathbf{r}_1)} \]

In order to evaluate the last integral, one must write the last term in body coordinates where the \( \mathbf{R}_i \)'s are constant in direction as well as magnitude. This is accomplished by using the relation (38, p. 247)

\[ e^{i \mathbf{Q} \cdot \mathbf{R}} = 4 \pi \sum_{m} \frac{1}{Q^2} Y_m(\mathbf{Q}) Y_m(\mathbf{R}) \int \mathbf{d} \mathbf{Q} \mathbf{R} \]

(2.46)
along with Equation A3 which states
\[ \gamma_s^e \left( \hat{A}_z \right) = \sum_m D_{m'm'}^{\ell} (\alpha) \gamma_m^b \left( \hat{A}_z \right) . \]  

(2.48)

From Equation 2.12, we find that the rotational wavefunctions \( \Psi_{LM}(\alpha) \) can be written as
\[ \Psi_{LM}(\alpha) = \sqrt{\frac{2L+1}{8\pi^2}} \sum_{K} a_{N,K}^{L} D_{m,K}^L(\alpha) \]  

(2.49)

It should be recalled that the expansion parameters \( a_{N,K}^{L} \) depend on the asymmetry parameter only if we are describing the motions of an asymmetric rotor. For a symmetric or spherical rotor, the wavefunctions can be expressed in analytic form and the \( a_{N,K}^{L} \)'s are merely numbers that are determined from the symmetry of the alpha structure, as was shown in Section C.

The last integral of Equation 2.46 can then be evaluated with the aid of Equation C12
\[ \int d\alpha \psi_{LM'}^*(\alpha) \psi_{LM}(\alpha) \sum_{\alpha'} e^{iQ \cdot \hat{R}_2} = 4\pi \sum_{m,m'} a_{N,K'}^{L',*} a_{N,K}^{L} \gamma_m^b(\hat{A}_z) \]  

(2.50)

Since we are concerned only with even-even nuclei, all initial spins will have spin \( 0^+ \). Therefore, in order to shorten the remaining calculations, we set \( L=0 \), and proceed with this specialized case. The integral then simplifies to
By using the identity
\[
\begin{pmatrix}
  i & j & 0 \\
  -m & m & 0
\end{pmatrix} = \frac{(-1)^{r+m}}{\sqrt{2r+1}}
\]
and Equations 2.46 and 2.51, the matrix element becomes
\[
\langle f | H' | i \rangle = \frac{4\pi Z e^2}{L^2 Q^2} \frac{F_0(Q)}{n} \sum_{k' \mu' k' h'} Y_{L'M'}^* (Q) \sum_{l''} \sum_{l'''} Y_{L'k'}^* (R_z') \mathcal{A}_{\mu' k' h'} \mathcal{A}_{l'' l'''} \mathcal{A}_L (Q R_z) \mathcal{A}_L (Q R_z) \mathcal{A}_L (Q R_z)
\]

In evaluating $|\langle f | H' | i \rangle|^2$, one must average over the initial states and sum over the final states. In the present case, $L=0$, so we need only sum over final states. Using the completeness relation of spherical harmonics (39, p. 69)
\[
\sum_{M'} \frac{Y_{L'M'}^* (Q)}{2 L' + 1} \frac{Y_{L'M'} (Q)}{2 L' + 1} = \frac{1}{4\pi}
\]
one can show this quantity to be
\[
|\langle f | H' | i \rangle|^2 = \left( \frac{4\pi Z e^2 F_0(Q)}{L^2 Q^2 n} \right)^2 \left| \sum_{k' \mu' k' h'} \sum_{l''} \sum_{l'''} Y_{L'k'}^* (R_z') \mathcal{A}_{\mu' k' h'} \mathcal{A}_{l'' l'''} \mathcal{A}_L (Q R_z) \mathcal{A}_L (Q R_z) \mathcal{A}_L (Q R_z) \right|^2
\]

Thus, the theoretical cross section for the CAP model can be written as
\[
\left( \frac{d\sigma}{d\Omega} \right)_{\text{point}} = \left( \frac{d\sigma}{d\Omega} \right)_{\text{point}} \left| F_{LN}^\mu \right|^2
\]
where the form factor $F_{LN}^\mu$ can be calculated from Equations 2.37, 2.42 and 2.54 to be
In Sections G and H, explicit form factors will be calculated for symmetric top structures. Since \(|K|\) is then a good quantum number, the form factor will be denoted by \(F_{\pi KK}\).

Most of the calculations in this paper will involve small momentum transfer (\(Q \leq 3\; \text{fm}^{-1}\)). In this limit \(\rho(r)\) can be approximated as a normalized gaussian function

\[
\rho_\sigma(\gamma^2) = \left(\frac{3}{2\pi\sigma^2}\right)^{\frac{3}{2}} e^{-\frac{3\gamma^2}{2\sigma^2}},
\]

and its Fourier transform then becomes

\[
F_\sigma(Q) = e^{-Q^2\sigma^2/6},
\]

where \(\sigma\) is the root mean squared (rms) radius of each alpha cluster. The interactions between alpha clusters may cause their rms radii to be slightly larger than the 1.63 fm valid for the \(^4\text{He}\) nucleus (40). In the present calculations, the parameter \(\sigma\) was found to always lie between 1.7 and 2.0 fm.

F. Electromagnetic Transition Matrix Elements

The partial mean width of a nuclear energy level decaying by multipolarity \((\lambda, \ell)\) between initial and final states of \((N,L)\) and \((N',L')\) is (41, p. 271)

\[
\Gamma_{\lambda, \ell}^{N,L; N',L'} = \frac{8\pi(\ell+1)}{3(2\ell+1)!} \left(\frac{E_{\ell}}{\tilde{E}_{\lambda}}\right)^{2\ell+1} B(\lambda; N', L' \rightarrow N, L),
\]

where \(\lambda\) will be either \(E\) or \(M\) depending upon whether the radiation is electric or magnetic, and \(\ell\) is the order of the transition. The last term in
the above equation is the reduced transition probability which in our notation is

$$B(\ell; N' \leftarrow N) = \frac{1}{2L+1} \sum_{M'_{m} M_{m'}} \left| \langle N'L'M' | \frac{\alpha}{2 \pi} \lambda_{\ell m}^{(s)} | NLm \rangle \right|^2. \quad (2.60)$$

The quantity $\sum_{m} \lambda_{\ell m}^{(s)}$ represents the electric or magnetic multipole operator of rank $\ell$ expressed in laboratory coordinates, and the sum $\sum_{M_{m}}$ arises since the quantity must be averaged over the initial and summed over the final states. The sums over the magnetic quantum numbers can be carried out by using the Wigner-Eckart theorem of Equation C18

$$\langle N'L'M' | \frac{\alpha}{2 \pi} \lambda_{\ell m}^{(s)} | NLm \rangle = (\frac{\alpha}{2 \pi})^{L-M} \left( \begin{array}{ccc} L' & L & \ell \\ -M & M & m \end{array} \right) \langle N'L' || \lambda(\ell) || NL \rangle, \quad (2.61)$$

and the unitarity relations of the 3-J symbols (Equations C6 and C7). The reduced transition probability is then

$$B(\ell; N' \leftarrow N) = \frac{1}{2L+1} \left| \langle N'L' || \lambda(\ell) || NL \rangle \right|^2. \quad (2.62)$$

The operators $\lambda_{\ell m}^{(s)}$ are evaluated in the long wavelength approximation as

$$E_{\ell m}^{(s)} = \frac{\alpha}{2 \pi} \int d^3 \tau \rho_N(\tau) \gamma^2 \gamma_{\ell m}(\phi, \varphi) \quad (2.63)$$

and

$$M_{\ell m}^{(s)} = -\frac{\alpha}{c (\ell+1)} \int d^3 \tau \gamma^2 \frac{\gamma}{\gamma^2} \gamma_{\ell m}(\phi, \varphi) \chi_{\ell m}(\tau), \quad (2.64)$$

where $\rho_N(\tau)$ and $j_N(\tau)$ represent the charge density and current density inside the nucleus, and the integration is carried out over the finite volume of the nucleus. These operators can be shown to be tensors of rank $\ell$ (43, p. 35), so from Equation C20 we find
The last term, $\lambda^{(b)}_{\ell m}$, is the corresponding intrinsic multipole moment of the $\alpha$-structure in body coordinates and is the quantity which induces the transition.

Again, we shall consider only transitions between states of the ground state rotational band so that the wavefunctions are of the form

$$| N L M \rangle = \sqrt{\frac{2 L + 1}{8 \pi^2}} \sum_{K} a_{N K}^L D_{M K}^L (\alpha) .$$

(2.66)

The matrix element involved in the transition can be evaluated by using Equations 2.61, 2.66 and C12 along with some symmetry relations of the rotation matrices:

$$\sqrt{\frac{2 L + 1}{4 \pi}} < N' L' M' | \lambda^{(s)}_{\ell m} | N L M >$$

$$= \sqrt{\frac{(2 L' + 1)(2 L + 1)(2 L + 1)}{4 \pi}} \sum_{K' H'} \frac{a_{N' H'}^L a_{N K}^L}{8 \pi^2} \int d \alpha_1 D_{m_m'}^{L m} D^{L m'}_{m m'} D_{N K}^{L m} \lambda^{(b)}_{\ell m} .$$

(2.67)

The reduced matrix element of Equation 2.61 can then be written as

$$< N' L' | 2 L (\alpha) | N L > = \sqrt{\frac{(2 L' + 1)(2 L + 1)(2 L + 1)}{4 \pi}} \sum_{K' m' K} (-)^{L' + K'} a_{N' H'}^L a_{N K}^L \left( -\frac{L' \times L}{m'} \right) \lambda^{(b)}_{\ell m} .$$

(2.68)

This relation will be used extensively in the next two sections in order to extract theoretical multipole moments from the experimental values of $(N' L' \parallel \lambda^{(b)} \parallel N L)$. 

$$\lambda^{(s)}_{\ell m} = \sum_{m} D_{m m}^{L} (\alpha) \lambda^{(b)}_{\ell m} .$$

(2.65)
The intrinsic multipole moments of the $\alpha$-structure, $\lambda_m^{(b)}$, can be found from Equations 2.63 and 2.64, if the integrations are carried out in body coordinates. Most of the transitions in deformed even-even nuclei are caused by the intrinsic electric multipole moments, so these quantities will be evaluated first. The nuclear charge density will be the same as that assumed in Equation 2.32 and is

$$\rho (x, R^2) = 2 e \sum_{i=1}^{n} \rho_o \left| x - R_i \right|.$$  \hspace{1cm} (2.69)

The integral in Equation 2.63 can then be evaluated by noting that in its derivation, one only considers those fields outside of the nuclear charge distribution (39, p. 99). Since the electric field outside of a spherical charge distribution is the same as if the charge were centered at the center of mass, we can instead use the density

$$\rho (x, R^2) = 2 e \sum_{i=1}^{n} S \left| x - R_i \right|.$$  \hspace{1cm} (2.70)

The integral in Equation 2.63 then becomes

$$E_{\lambda m}^{(b)} = 2 e \sqrt{\frac{9 m}{2 \lambda + 1}} \sum_{i=1}^{n} R_i^{\lambda} \chi_{\lambda m} (\theta_i, \phi_i),$$  \hspace{1cm} (2.71)

an expression independent of the rms radius of each alpha cluster.

The magnetic intrinsic moments are somewhat more difficult to determine because the current density $j(r)$ must be known at every point inside the nucleus. In Section 1, it will be shown that the rotation of an $\alpha$-structure is not rigid and only a fraction of the nuclear mass contributes to the overall rotation of the configuration. Therefore, within the framework of the present model, it is virtually impossible to find a value for the intrinsic magnetic moment that is more accurate than the one which can be
calculated by assuming that the alpha clusters are point particles. However, magnetic transitions appear in only a few isolated cases for light $A=4N$ nuclei, so we shall be satisfied in making such an approximation. With this assumption, the form of the intrinsic magnetic moments, $M_{2m}^{(b)}$, is the same as that obtained by considering the orbital contribution of the nucleons in a shell model calculation and may be written as (42)

$$M_{2m}^{(b)} = \mu_N g_\alpha \frac{2}{2+1} \frac{2}{\rho} \sum_p \Gamma_{2m}^{(b)} (\theta_p, \phi_p) \left[ \gamma_p \frac{2}{2m} \right], \quad (2.72)$$

where $\mu_N = \frac{e^2}{4mc}$ is the nuclear magneton, $g_\alpha = 0.500$ is the gyromagnetic (or charge to mass) ratio of each alpha particle, and $\frac{2}{2m}$ is the orbital angular momentum of the $p^{th}$ cluster. By introducing pseudospherical coordinates and using Equation C17, we find

$$M_{2m}^{(b)} = \mu_N g_\alpha \frac{2}{2+1} \frac{2}{\rho} \sum_p \Gamma_{2m}^{(b)} (\theta_p, \phi_p) \left[ \gamma_p \frac{2}{2m} \right] \quad (2.73)$$

The above expression can be easily evaluated for magnetic dipole moments because

$$\sum_p \gamma^0 (L_p) \gamma \theta \phi = \frac{1}{4\pi} \frac{1}{4\pi} L \cdot \tau, \quad (2.74)$$

where $L_t$ is the $t^{th}$ component of the total angular moment of the $x$-structure, $L$. The dipole operator may then be calculated as

$$M_{1m}^{(b)} = \frac{3}{2} \mu_N \frac{2}{2+1} \frac{2}{\rho} \sum_p \left[ \gamma_p \frac{2}{2m} \right] \frac{L_t}{4\pi} \frac{L_m}{4\pi} = \frac{3}{2} \frac{1}{4\pi} L \cdot \tau \quad (2.75)$$

It can be shown that the above expression arises whenever the ratio of the charge current density to mass current density is $\frac{1}{2}$ for every point inside.
the nucleus. The Nilsson model predicts

\[ M^{(b)}_{\ell m} = \left( \frac{2}{\hbar^2} \right) \mu_n \sqrt{\frac{3}{4\pi}} L_m \]  

(2.76)

for this quantity, which of course gives the same value as the CAP model for the \( A=4N \) nuclei we are considering. From Appendix D, we find that the operator \( L_m \) can only change the magnetic quantum number of the wavefunction \( \langle NLM | \) ; so the CAP model, as well as the Nilsson model, predicts all magnetic dipole transitions between different rotational energy states to be identically zero.

Higher order magnetic multipole moments are more difficult to estimate because the sum cannot be evaluated in any simple fashion. In order to evaluate general matrix elements of the operator in Equation 2.73, we must express the angular momentum operators of each particle \( (L_p)_t \) in terms of the total angular momentum of the structure. Such a relation will depend not only on the shape of the \( \alpha \)-structure, but also on the approximations that must be made concerning the rotation of the nuclear mass. If one assumes the \( \alpha \)-structure to be rigid, the necessary relations can be found in a straightforward, but long and tedious classical calculation. For the present, however, we simply state the above discussion formally as

\[ (L_p)_t = \sum_{\ell,\ell'} A_{\ell\ell'}^p L_{\ell'} \]  

(2.77)

and by combining this expression with Equation 2.73, we obtain

\[ M^{(b)}_{\ell,m} = \left( \frac{2 \ell + 1}{2\ell + 1} \right) \sum_{\ell'} \sum_{m'} \frac{1}{\ell'} \frac{\ell + m'}{\ell - m'} \begin{pmatrix} \ell & \ell & \ell - 1 \\ \ell & m & -m' \end{pmatrix} \frac{\tilde{\tau}_{\ell,\ell'} \tilde{\gamma}_{\ell',m',m}(\Theta_p, \Phi_p) A_{\ell\ell'}^p}{\tilde{\tau}_\ell} \]  

(2.78)

From this last equation, we see that all magnetic multipole operators, \( M_{\ell m}^{(b)} \),
are linear combinations of the three angular momentum operators $L_1$, $L_0$, $L_{-1}$. Thus, the CAP model, under the approximations made, will predict a zero value for all multipole orders of magnetic transitions. In Section H, it will be shown that such a definite prediction is consistent with the several magnetic transitions that have been observed among the low-lying states of several light $A=4N$ nuclei. It is interesting to note that the asymmetric rotor yields a similar prediction for magnetic octopole transitions, since the operator for this model has been previously shown to be (43, p. 56)

$$M_{3m}^{(b)} = \mu_n \left( \frac{2}{A} \right) \frac{2\pi}{3} R_0^2 L_m$$ \hspace{1cm} (2.79)

where $R_0$ is the average radius of the deformed nucleus.

Unlike the mean lifetime of a nuclear state, the reduced transition probability is independent of the energy of the emitted photon (see Equations 2.59 and 2.60) and is therefore the usual theoretical quantity that one compares with experiment. In addition, this quantity is normally expressed in dimensionless Weisskopf units as

$$|M|_{\text{w.u.}}^2 = \frac{B(\lambda \ell; \lambda' \ell' + \kappa \ell' \ell)}{B_{\text{s.p.}}(\lambda \ell)}$$ \hspace{1cm} (2.80)

where $B_{\text{s.p.}}(\lambda \ell)$ is an approximate value for the single-particle reduced multipole transition and is defined to be (44)

$$B_{\text{s.p.}}(E \ell) = \frac{1}{4\pi} \left( \frac{3}{2+\epsilon} \right)^2 (1.2)^{2.3} A^{2.3/3} \left[ e^{2 \epsilon} m^{2.2} \right]$$ \hspace{1cm} (2.81)

$$B_{\text{s.p.}}(M \ell) = \frac{10}{4\pi} \left( \frac{3}{2+\epsilon} \right)^2 (1.2)^{2.3} A^{(2.3/2)/3} \left[ \mu^2 + m^{2.2} \right]$$ \hspace{1cm} (2.82)
Usually, the enhanced E2 transitions for deformed nuclei in the 2s-1d shell have a value of $|M^2|_{\text{w.u.}}$ between 10 and 50. Several comparisons between the experimental and theoretical transitions will be made in the next section.

In some calculations, it is advantageous to work with the reduced matrix elements $\langle N' L' | \lambda \alpha \rangle _{NL}$ rather than the $B(\lambda \alpha; L'\rightarrow L)$. From Equation 2.62, one sees that only the absolute value of this quantity can be obtained from experiment. One additional reduced matrix element that can be experimentally measured for even-even nuclei is the static quadrupole moment of the first $2^+$ excited state (denoted $Q_2^+$). The technique for measuring this quantity has only been perfected within the last few years, but already it has been used to determine $Q_2^+$ for a number of light even-even nuclei. From the definition of a static quadrupole moment,

\[
Q_2^+ = \langle J, M=J, \pi' \mid Q_{20} \mid J, M=J, \pi \rangle ,
\]

we can readily relate this quantity to the corresponding reduced matrix element as follows:

\[
Q_2^+ = \sqrt{\frac{4\pi}{2\ell+1}} \left| \left\langle J, M=J, \pi' \mid \sqrt{\frac{2J+1}{4\pi}} E_{20} \mid J, M=J, \pi \right\rangle \right| ^2
\]

\[
= \sqrt{\frac{16\pi}{5}} \left( \begin{array}{cc} J & 2 \\ -J & 0 \end{array} \right) \left( \begin{array}{c} J \\ 0 \end{array} \right) \langle J \pi' \parallel E(2) \parallel J \pi \rangle .
\]

The multiplicative constant $\sqrt{\frac{16\pi}{5}}$ is needed in order for our quantities to be consistent with those most commonly used. Some authors will define the reduced matrix element as the negative of our value. When $J=2^+$, we find

\[
Q_2^+ = \sqrt{\frac{2\pi}{7}} \langle 2^+ \parallel E(2) \parallel 2^+ \rangle .
\]

It should be noted that this last measurement is capable of producing the
sign as well as the magnitude of the reduced matrix element, and this fact will be used later to determine the quadrupole shapes for several light $A=4N$ nuclei in the 2s-1d shell.

G. Review of 1P Shell Nuclei

1. The limited success of the CAP model for 1p shell nuclei

As noted in the introduction, Wheeler (7) was the first person to discuss the theoretical energy spectra for the most plausible $K$-structures of $^8$Be, $^{12}$C, and $^{16}$O, namely the dumbbell, equilateral triangle, and regular tetrahedron respectively. Since very little was known at that time about the experimental levels of these nuclei, he simply made some reasonable estimates for the vibrational and rotational constants and presented his calculated levels so that they could be either verified or repudiated by future experiments. To show that he was completely honest in finding values for his constants, Wheeler then compared his results with one of the few observables available at that time. This quantity was the position of the first energy level of $^8$Be at 3 MeV which he incorrectly predicted at 2 MeV. This large discrepancy did not discourage him in the least, since it merely indicated that the rotational and vibrational constants would have to be taken as fitting parameters to be determined at a later time when more levels were discovered.

Since Wheeler's original work, the CAP model has been thoroughly investigated for the 1p shell nuclei and found to be somewhat limited in its application (19-21). Figure 2.7 shows the best agreement attainable between the experimental and theoretical energy levels for these three nuclei. The values used for the rotational and vibrational parameters are given in Table
Figure 2.7. Level schemes of $^8$Be, $^{12}$C, and $^{16}$O, and comparison with the CAP model.

Table 2.9. Values of parameters used in fitting the observed levels.

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>Rotational parameters (MeV)</th>
<th>Excitation energy (MeV) and symmetry classification of normal vibrations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^8$Be</td>
<td>$A_1=A_2=.48$ $A_3=?$</td>
<td>$?; (A_1)$ --- ---</td>
</tr>
<tr>
<td>$^{12}$C</td>
<td>$A_1=A_2=.74$ $A_3=.82$</td>
<td>7.7; ($A_1'$) 8.4; ($E'$) ---</td>
</tr>
<tr>
<td>$^{16}$O</td>
<td>$A_1=A_2=A_3=.5i$</td>
<td>6.05; ($A_1$) 6.77; ($E$) 4.7; ($F_1$)</td>
</tr>
</tbody>
</table>
2.9. The apparent agreement between experiment and theory is somewhat superficial since the number of fitting parameters is about equal to the number of levels predicted by theory. Also, some noticeable inconsistencies occur when certain reduced transition matrix elements are calculated and compared with experiment. It is encouraging to note, however, that all \( \alpha \)-structures for \(^{12}\text{C}\) and \(^{16}\text{O}\), other than the two logical ones assumed in Figure 2.7 can be eliminated as being the physical structure because they predict too many low-lying levels. Some examples of these alternate structures are the isosceles triangle for \(^{12}\text{C}\) (\(C_{2v}\) symmetry), the planar rhomboid for \(^{16}\text{O}\) (\(D_{2h}\) symmetry), etc. Also, some of the discrepancies of the CAP model concerning the reduced matrix elements have been rectified by considering a more realistic \( \kappa \)-particle model. Therefore, because of its relevance to the present research, a review of this past work will be presented for each of the three nuclei. It will be found that such a review will also enable us to gain new insight into the validity of some of the approximations made earlier during the derivation of the CAP Hamiltonian.

2. The dumbbell rotor for \(^8\text{Be}\)

The dumbell structure for \(^8\text{Be}\) has \(D_{2h}\) symmetry, and by methods analogous to Section C, one can show that the rotational states belonging to the completely symmetric IR are

\[
\mathcal{L}_K^{T} = 0^+_0, 2^+_0, 4^+_0, 6^+_0, \cdots.
\]  

(2.86)

Since nonzero values of \(K\) do not exist, the Hamiltonian for the ground state rotational band is simply

\[
\mathcal{H} = \mathbf{\hat{A}}_1 \cdot \mathcal{L}(\mathcal{L}+1).
\]  

(2.87)
The physical concept of parity for this linear structure is easily understood, because the inversion operation merely permutes the two alpha particles and is therefore equivalent to any 2-fold rotations about an axis in the xy plane. From Equation B7, one then finds

\[ I \ D_{M0}^L (\alpha) = (-)^L D_{M0}^L (\alpha) \]  

(2.88)

This agrees with Equation 2.86 which was found purely from mathematical formalism. The theoretical levels are shown in Figure 2.7a with the rotational parameter arbitrarily chosen to be \( A_1 = 0.48 \) MeV. The theoretical reduced \( \chi \)-widths are predicted by a simple extension of the CAP model proposed by Davis (45, p. 67; 46, p. 313) which need not be considered at present.

The experimental states above 16 MeV cannot be explained by the CAP model and are now believed to be caused by one of the alpha clusters breaking up into its constituents, such as nucleons, deuterons, tritons, etc. (47).

If one considers the rotor to execute rigid motion, the rotational parameter \( A_1 \) can be related to the dimensions of the \( \chi \)-structure by the classical relation

\[ I_i = \frac{\hbar^2}{2 \alpha_i} = m_\chi (\frac{d^2}{2} + \frac{4}{3} \alpha^2) \]  

(2.89)

where \( m_\chi \) and \( a \) are the mass and rms radius of each alpha particle, and \( d \) is the distance between the centers of the two clusters. Assuming a realistic value for \( a \) of 1.7 fm (see Section E), one calculates the separation distance to be \( d = 3.7 \) fm. In the last section of this chapter, it will be shown that only a fraction of the nuclear matter contributes to the moment of inertia for most deformed nuclei. Therefore, the value \( d = 3.7 \) fm should only be taken as a lower limit to the actual separation.
Another estimate of the alpha separation distance can be made by plotting the various phenomenological $\alpha-\alpha$ potentials which are derived from $\alpha-\alpha$ scattering and locating the minimum in the potential. One of the most common $\alpha-\alpha$ potentials in use today is that of Afzal et al. (48) which is found to be dependent on the angular momentum $l$ of the composite nucleus. The minimum of the $L=0$ potential is approximately $d=2.9$ fm. Due to the strong repulsive force of this potential at small distance, this value may again be smaller than the actual alpha separation distance by at least 0.5 fm (49, p. 462; 50).

Unfortunately, no experimental information exists for the electron scattering form factors or the reduced electric transitions of the rotational states of $^8$Be, since these levels disintegrate immediately into two alpha particles. Such information, however, does exist for $^9$Be, and a unified version of the $\alpha$-particle model predicts an alpha separation distance of about $d=3.8$ fm for this nucleus, as will be briefly discussed in Chapter IV.

3. $^{12}$C and the RAP model

Figure 2.7b shows the energy levels of $^{12}$C assuming that its $\alpha$-structure has $D_{3h}$ symmetry. The levels can be calculated from the formula

$$H = \mathcal{A}_1 L(L+1) + K^2(A_3-A_1) + \gamma_1 \hbar \omega_1 + \gamma_2 \hbar \omega_2,$$

where the rotational and vibrational parameters are given in Table 2.9.

These values differ somewhat from those obtained in a 1953 calculation (21) because at that time the spin of the $3^-$ level at 9.64 MeV was not known. The allowed rotational bands for the two normal vibrations can be found from Table 2.1. Since the $\alpha$-structure under consideration is planar, the parity
of the levels can again be determined by rotational motion only. In the present case, the inversion operation is now equivalent to a 2-fold rotation of the structure about the z axis, and so from Equation B6 one finds

$$I \ D_{MK}^{L} (\alpha) = (-)^{K} D_{MK}^{L*} (\alpha) .$$

(2.91)

The agreement between this last equation and the previous mathematical formalism can only be appreciated when one notes that all possible vibrational modes of the triangular structure, no matter how many phonons of the two normal vibrations of Equation 2.90 are considered, belong to only three of the six IR's of $D_{3h}$, these being $A_{1}^{'}, A_{2}^{'},$ and $E^{'}. From Table 2.1, we see that all rotational states belonging to these three IR's have parity $(-)^{K}$.

The elastic scattering cross section predicted by the triangular $\alpha$-structure can be calculated from Equation 2.56. The resulting formula is

$$F_{oo}^{+} = F_{\alpha}(q) \ j_{0}(qR),$$

(2.92)

where $F_{\alpha}(q)$ is the experimental form factor of each alpha particle, R is the radial distance of each alpha cluster from the center of mass of the triangle, and q is the electron momentum transfer. The best agreement with experiment (51) is shown by the solid line in Figure 2.8, and occurs when the parameter R is chosen to be $R=1.75$ fm. This corresponds to a separation distance between adjacent alpha particles of $d=3.03$ fm.

Other values for this separation distance can be obtained from the experimental electric transitions probabilities observed from the $2^{+}(4.43$ MeV) and $3^{-}(9.64$ MeV) excited states to the $0^{+}$ ground state. Both of the excited states are explained by the CAP model as being rotational states of the zero-point vibrational mode, and have the following rotational wavefunctions
Figure 2.8. The square of the experimental elastic form factor is plotted along with the curves predicted by the CAP model (with one variable) and the RAP model (with no variable). The one parameter in the CAP model gives the alpha separation distance of $d=3.03\ \text{fm}$.

Figure 2.9. The absolute value of the elastic form factor is plotted along with the curve predicted by the CAP model. The one parameter yields an alpha separation distance of $d=3.36\ \text{fm}$. 
By applying Equation 2.71 to the triangular structure, we find that the intrinsic moments are related to the radial distance \( R \) by the formulas

\[
Q_{20} = 2 \ E_{20} = -6 \ e R^2
\]

\[
E_{33} = -E_{3,-3} = -\frac{3}{2} \sqrt{5} \ e R^3
\]

The most reliable values for the experimental reduced transition probabilities of these two excited states are \(44\)

\[
B \ (E 2^+; \ 2^+ \rightarrow 0^+) = 8.5 \pm 0.65 \ e^2 \frac{e}{m^4}
\]

and

\[
B \ (E 3^-; \ 3^- \rightarrow 0^+) = 11.2 \pm 2.5 \ e^2 \frac{e}{m^6}
\]

which correspond to the reduced matrix of (see Equation 2.62)

\[
\begin{vmatrix} 6.5 \pm 0.2 \ e \frac{e}{m^2} \end{vmatrix}_{\exp}
\]

and

\[
\begin{vmatrix} 28 \pm 3 \ e \frac{e}{m^3} \end{vmatrix}_{\exp}
\]

From Equations 2.68, 2.93, and 2.94, we find that the theoretical reduced matrix elements can be expressed as

\[
\begin{vmatrix} \frac{5}{\sqrt{16 \pi}} \ \left| \begin{pmatrix} 0 & 2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right| Q_{20} \end{vmatrix}_{\text{theor}}
\]

and

\[
\begin{vmatrix} \frac{7}{\sqrt{2 \pi}} \ \left| \begin{pmatrix} 0 & 3 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right| E_{33} \end{vmatrix}_{\text{theor}}
\]
The magnitudes of the intrinsic moments can now be calculated from the last four equations and are

\[ |Q_{20}| = 20.6 \pm 0.6 \text{ fm}^2 \]  
\[ |E_{33}| = 26.5 \pm 2.8 \text{ fm}^3 \]  

Equating these values with Equations 2.95 and 2.96, one finds the two values for the radial distance to be \(1.8 < R < 1.9\) fm for the quadrupole transition, and \(1.9 < R < 2.0\) fm for the octopole transition. These values are noticeably larger than the \(R=1.75\) fm found from the elastic electron scattering experiments. However, this is to be expected since centripetal distortions will pull the alpha clusters outward for excited states of nonzero spin (52).

The preceding results of the CAP model on \(^{12}\)C are quite good, but it is very discouraging that so many parameters are needed to correlate the low-lying states with theory. An alternate \(\alpha\)-particle model, which contains no fitting parameters, was formulated around 1960 and called the realistic \(\alpha\)-particle (RAP) model. In this model, the Hamiltonian for \(^{12}\)C was considered in the form

\[ H = \sum_{i=1}^{3} \frac{\hat{p}_i^2}{2m} + \sum_{i \neq j} V(\sqrt{i_j} - \sqrt{j_i}) \]  

where \(V(r)\) is one of several phenomenological potentials which can be derived from \(\alpha\)-\(\alpha\) scattering experiments (48). Usually, due to the complexity of the calculation, only static properties of the nucleus (such as the binding energy and rms radius of the ground state configuration) are computed. The numerical results of this model vary slightly depending upon which phenomenological potential is used (53). However, nearly all of the
calculations predict too small of a binding energy and too large of a rms for the ground state configuration. As one would expect, they are consistent in describing the ground state as a triangular structure much like that of the CAP model. In one recent paper, the elastic scattering cross section curve of the RAP model was plotted (as shown by the dashed curve of Figure 2.7) and found to be in poor agreement with experiment (51). By noting the position of the minimum in this curve at $q^2 = 2.1 \text{ fm}^{-2}$, one can compute the separation distance between adjacent alpha particles to be 3.8 fm. This is considerably larger than the value of $d = 3.0 \text{ fm}$ predicted earlier by the CAP model. In lieu of such discrepancies between experiment and theory, we are forced to conclude that a stronger $\alpha$-$\alpha$ force is needed in $^{12}\text{C}$ to pull the three alpha particles together. Further evidence supporting this illation can be found in a very recent paper (54), where the author attached a multiplicative strength parameter, $\lambda$, to the nuclear part of the phenomenological $\alpha$-$\alpha$ potential, and found that the correct binding energy was obtained with $\lambda = 1.4$.

One major variance between the CAP and RAP models for $^{12}\text{C}$ arises in their respective descriptions of the first excited $0^+$ state at 7.66 MeV. The CAP model depicts this state as the "breathing" vibration, (denoted by $\pi \omega_1$ in Table 2.9). On the other hand, the RAP model characterizes the state as being primarily a linear structure of three particles. Since the effective $\alpha$-$\alpha$ potential for $^{12}\text{C}$ is closer to that of the RAP model, the latter description is probably the more factual of the two. Therefore, we should not put too much emphasis on the rotational states that are assumed in the CAP model to be built on normal vibrations, since in reality they may be built on different $\alpha$-structures.
4. $^{16}_0$ - spherical or deformed?

Three years after Wheeler's original work, a molecular physicist by the name of Dennison further developed the tetrahedron model for $^{16}_0$ and found that the theoretical levels were consistent with the two experimental levels known at that time (19). Then in 1954, he re-examined the model and found very good agreement between the experimental and theoretical levels (19). Figure 2.7c shows his comparison for all states below 10.5 MeV. Dennison also succeeded in correlating most of the eleven additional experimental states observed at that time between 10.5 and 13.3 MeV. However, any agreement between theory and experiment in this region must be considered as coincidental, since the observance of isotopic spin $T=1$ states in this energy region indicate the presence of single particle states.

The CAP model has also been shown to explain the two diffraction minima in the observed electron scattering cross section in a very simple way (36). Using Equation 2.56 along with the tetrahedral structure sketched in Figure 2.7c, one obtains the same equation as was found for $^{12}_C$, namely

$$F_{00}^+ = F_\alpha(q) J_0(qR),$$

(2.106)

where $F_\alpha(q)$ is the experimental form factor of the alpha particle and $R$ is now the radial distance of each alpha cluster from the center of mass of the tetrahedron. Figure 2.9 shows the most recent comparison that has been made with experiment. It should be noted that the height of the second maximum in the cross section could be better predicted if a slight variation were allowed in rms radius of the alpha particles. By observing that the first diffraction minimum occurs at 1.52 fm$^{-1}$, we can easily compute the radial
distance to be \( R = 2.06 \text{ fm} \) which corresponds to a separation distance between alpha particles of \( d = 3.36 \text{ fm} \).

The radial distance can also be computed from the rotational parameter \( A_1 \). Using arguments much like those of Equation 2.77, we can compute the radial distance to be \( R = 1.0 \text{ fm} \). Since we have considered the tetrahedron to be a rigid rotor, this value should again be taken as a lower limit. Finally, we can also calculate the radial distance from the observed octupole transition of the \( 3^- (6.13 \text{ MeV}) \) state, which in the CAP model is a rotational state with the wavefunction

\[
\langle \alpha \mid 3^- \rangle = \sqrt{\frac{7}{8 \pi^2}} \left[ \sqrt{\frac{1}{2}} D_{m_2}^{3 \ast} (\alpha) - \sqrt{\frac{2}{2}} D_{m_2}^{3 \ast} (\alpha) \right]. \tag{2.107}
\]

The observed reduced transition matrix element is (44)

\[
B (E 3; 3^- \rightarrow 0^+) = 2.10 \pm 0.2 \text{ e}^2 \text{ fm}^6 \tag{2.108}
\]

Following the procedure used for \(^{12}\text{C}\), these last equations can be shown to predict a radial distance of \( R = 2.0 \pm 0.1 \text{ fm} \) which is disappointingly close to the value obtained from the elastic electron scattering data. One would have expected the value to be somewhat larger because of centripetal distortion.

The CAP model runs into additional difficulties when other reduced transitions are calculated. The main discrepancy arises in calculating the monopole transition of the \( 0^+ (6.06 \text{ MeV}) \) state. In the CAP model, this state is considered to be the dilational vibration and Kameny (20) found that the calculated transition matrix was four times larger than experiment. Noble reconsidered the problem in a somewhat different manner, but found essentially the same result (55). In fact, other authors have found that all
pure collective models which treat this state as a dilational mode of the entire nucleus will necessarily produce too large a matrix element by a factor of three or four (56, 57). Another transition which most likely cannot be explained by the CAP model is the enhanced E2 transition between the $2^+(6.92 \text{ MeV})$ and the $0^+(6.06 \text{ MeV})$ which has a Weisskopf transition strength of $|M|^2_{\text{w.u.}} = 17.2 \pm 3.7$ (44). In addition, there is now good reason to believe that the $0^+$, $2^+$, and $4^+$ states at 6.06, 6.92, and 10.36 MeV may be members of a deformed rotation band since enhanced E2 transitions have observed between these three states (58, 59). The CAP model assumes these three states belong to rotational states of three different vibrational modes and therefore could not account for the large values observed for such transitions.

As in $^{12}$C, it appears that some of the deficiencies of the CAP model for $^{16}$O can be corrected by considering the appropriate RAP model. As far as I am aware, only one attempt has been made so far to solve such a 4-body problem (60). In solving the problem, the authors used a variational calculation which necessitated some rather drastic approximations. Nevertheless, the results are very interesting and should be stated. The ground state is still quite similar to that of the tetrahedron, and the separation distance of alpha particles is $d=3.4 \text{ fm}$, the same as that found in the CAP model from electron scattering data. The excited $0^+$ state, however, is found in this model to be a planar rhomboid, and the calculated monopole matrix element between the two $0^+$ states is only twice as large as experiment. It should be emphasized that the above results need further study. An alternate method of solving this problem, which in principle could be carried out exactly, is mentioned in Chapter V.
5. A critical review on the validity of the CAP model

From the preceding discussion on $^{12}$C and $^{16}$O, it appears that the CAP model is assured of giving a plausible description only to the rotational levels assumed built on the zero-point vibrational mode. Therefore, in considering possible structures for other $A=4N$ nuclei, we should not put too much emphasis on the rotational states that are explained in the CAP model as being built on normal vibrations, since in reality they may belong to different $\alpha$-structures. This viewpoint is also supported by a recent $\alpha$-cluster calculation which indicates that several $\alpha$-structures are in fairly close competition for the ground state configuration of $^{16}$O (59). Even with this limitation, it will be shown in the next section that unique $\alpha$-structures can be found for a number of $A=4N$ nuclei in the 2s-1d shell. Furthermore, it is very probable that the above restriction is too severe, and that we should only be careful with our interpretation of states built on the dilatational vibration. Therefore, in lieu of this latest, somewhat optimistic assumption, we shall continue to correlate observed high-lying rotational states with those allowed by various normal vibrations of the assumed $\alpha$-structure, and simply remember that under some circumstances such efforts may be purely an academic exercise with little physical meaning.

One encouraging point of the past review, however, is that the attractive part of the $\alpha-\alpha$ potential realized in nuclei with three or more alpha particles seems to be greater than that of the phenomenological potentials determined from $\alpha-\alpha$ scattering. Even if this strengthening results from the exchange of nucleons among alpha clusters we would still expect the symmetry relations of the CAP model to hold. In fact, Herzenberg (61) and Brink (62) both have shown that these symmetry conditions still apply for the two
types of microscopic cluster models noted earlier in the historical review. The main effect of this interchange should therefore be beneficial to the CAP model in that it would add to the total rigidity of the $\alpha$-structure.

H. Results for $A=4N$ Nuclei in the 2s-1d Shell

1. Previous work

Unlike the 1p shell nuclei, several reasonable $\alpha$-structures are possible for each $A=4N$ nucleus in the 2s-1d shell. In the early days of the CAP model, theorists were not able to select the correct structure from the available experimental data, and so they simply assumed that the physical structures were those which had the greatest number of bonds among adjacent alpha clusters. These configurations turned out to be bipyramids with all but two of the alpha particles forming a regular polygon in the equatorial plane. The only experimental evidence available for comparison at that time was the binding energies of these nuclei, and these quantities agreed quite well in theory (4,10). However, quite recent calculations of the electron scattering form factors using these bipyramidal shapes have shown that they are in rather poor agreement with experiment (34,35). Furthermore, nonbipyramidal shapes have been shown to yield better agreement with the observed energy levels (23,24). Since the time of these calculations, much additional experimental information has been obtained; so it was felt that all possible configurations for the $4N$ nuclei in the 2s-1d shell should be reconsidered. The rest of this section presents the results of such research.
2. Determining quadrupole shapes from experimental data

All of the configurations considered in this section will be either symmetric or slightly asymmetric tops. With this assumption one can readily find the approximate quadrupole shapes of some of the nuclei under consideration by relating the intrinsic quadrupole moment $Q_{20}$ to the two different experimental reduced matrix elements shown in the second and third columns of Table 2.10. The first matrix element, $\langle 2 \| E(2) \| 2 \rangle$, is found from the measured static quadrupole moment by means of Equation 2.85 while the other, $\langle 2 \| E(2) \| 0 \rangle$, is computed directly from the experimental reduced transition probability through Equation 2.62. The necessary theoretical relationship that one needs to calculate $Q_{20}$ follows from Equation 2.68 and noting that the levels involved belong to the ground state $K^T=0^+$ band so that

$$a_{NK}^L = s_{K0}^L.$$ The result is then simply

$$Q_{20} = 2E_{20} = \sqrt{\frac{16 \pi}{5 (2L'+1)(2L+1)}} \frac{\langle L' \| E(2) \| L \rangle}{\langle \ell \| \ell \| \ell \rangle}.$$ \hspace{1cm} (2.109)

From Equations 2.85 and 2.109, one finds the following simple relation between $Q_{20}^+$ and $Q_{20}$:

$$Q_{20}^+ = -\frac{2}{7} Q_{20} \hspace{1cm} (2.110)$$

The experimental ratio $B(E2, 4^+ \rightarrow 2^+)/B(E2, 2^+ \rightarrow 0^+)$ is shown in column six. Discrepancies between these values and the theoretical ratio of 10/7 (for the symmetric top) indicate that collective vibrations or single particle effects are of some importance in these low-lying states and help explain the slightly different answers obtained in columns four and five. Nevertheless, the results definitely show that $^{20}\text{Ne}$, $^{24}\text{Mg}$, and $^{32}\text{S}$ are highly
Table 2.10. Values for the intrinsic quadrupole moment of various nuclei as calculated from two different experimental reduced matrix elements.

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>Experimental Reduced Matrix Elements ( (\text{e fm}^2) )</th>
<th>Corresponding Intrinsic Quadrupole Moments (-Q_{20} (\text{fm}^2)) (From Column 2)</th>
<th>Experimental (B(E2; 4^+ \rightarrow 2^+))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^{20}\text{Ne})</td>
<td>(-32 \pm 4^a) (\langle 2</td>
<td></td>
<td>E(2)</td>
</tr>
<tr>
<td>(^{24}\text{Mg})</td>
<td>(-33 \pm 5^c,d) (\langle 0</td>
<td></td>
<td>E(2)</td>
</tr>
<tr>
<td>(^{23}\text{Si})</td>
<td>(+21 \pm 5^f,g,h) (\langle 2</td>
<td></td>
<td>E(2)</td>
</tr>
<tr>
<td>(^{32}\text{S})</td>
<td>(-26 \pm 8^f) (\langle 0</td>
<td></td>
<td>E(2)</td>
</tr>
</tbody>
</table>

^e Endt and Van der Leun, Nucl. Phys. 105, 1 (1967). (67)
prolate while $^{28}$Si is oblate. This information is of great help in formulating structures for these nuclei.

3. **Is $^{20}$Ne an internal rotor?**

The experimental spectrum of $^{20}$Ne shows a definite $K^\pi=2^-$ band beginning at 4.97 MeV. As has been noted previously (24), the only rigid $\alpha$-structure that can predict this band is the $D_{2d}$ distorted tetrahedron (Figure 2.10a). But in this model, the upper and lower dumbbell structures are separated by a relatively large distance, so they can rotate about the z axis in opposite directions. The amount of such motion would depend upon the height and width of the potential barrier opposing free internal rotation. So, besides reviewing the results of the $D_{2d}$ distorted tetrahedron, we will account for this "tunneling" effect (19,27) by considering the more realistic nonrigid structure of Figure 2.10b. The most popular $\alpha$-structure for $^{20}$Ne has been the $D_{3h}$ trigonal bipyramid (22,27,34,59,62) of Figure 2.10c. Since this structure incorrectly predicts a low-lying $K^\pi=3^-$ band (c.f. Table 2.1), it will not be considered further.

Figure 2.11 compares the predicted levels of the $D_{2d}$ distorted tetrahedron with experiment. Since this structure is that of a symmetric top, the exact formulae for the rotational energies may be taken from Equation 2.6. The symmetries of the nine intrinsic normal vibrations are given in Table 2.11 along with the calculated energies and rotational parameters for the vibrations believed to be observed in the experimental spectrum. In some cases, only a lower limit is given for $A_3$. The parameter $A_3$ must be at least this large in order to push certain theoretical levels that are not experimentally observed above 10 MeV.
Figure 2.10. Three of the most plausible configurations for $^{20}\text{Ne}$. 

(a) $D_{2d}$ DISTORTED TETRAHEDRON  
(b) $D_{2d}$ INTERNAL ROTATOR  
(c) $D_{3h}$ TRIGONAL BIPYRAMID
Figure 2.11. Comparison of the experimental levels of $^{20}\text{Ne}$ with the theoretical levels predicted by the $D_2d$ structure. The levels built on the zero-point vibrational mode can be better predicted if different values of $A_1$ are assigned for the $K=0$ and $K=2$ bands. Note that the scale is changed at 7 MeV for clarity.
Table 2.11. Possible normal vibrations for the $D_{2d}$ distorted tetrahedron structure of $^{20}\text{Ne}$. The symmetry of the double vibration is found by taking the direct product $B_2 \otimes B_2$.

<table>
<thead>
<tr>
<th>Frequency</th>
<th>$\omega_1$</th>
<th>$\omega_2$</th>
<th>$\omega_3$</th>
<th>$\omega_4$</th>
<th>$\omega_5$</th>
<th>$\omega_6$</th>
<th>$\omega_7$</th>
<th>$\omega_8 \sim 2\omega_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rotational Parameters (MeV)</td>
<td>$A_1 = A_2$</td>
<td>0.20</td>
<td>0.12</td>
<td>0.11</td>
<td>-</td>
<td>0.15</td>
<td>0.17</td>
<td>-</td>
</tr>
<tr>
<td>$A_3$</td>
<td>1.0</td>
<td>$\geq 0.76$</td>
<td>$\geq 0.64$</td>
<td>-</td>
<td>0.93</td>
<td>$\geq 0.32$</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
Nearly all levels below 10 MeV are well explained as rotational states built on the allowed normal vibrations. The explicit K=0 bands have long been known; indeed, our level assignments are similar to those arising from other collective models (72,73). The third K=0^+ band beginning at approximately 8.7 MeV is built on a double vibration of \( \omega_4 \). This interpretation is supported by the high reduced alpha widths (\( \approx 1300 \) KeV) observed for levels of this band (72). The excitation energy of this of this vibration should be somewhat less than \( 2\hbar \omega_4 \) because of anharmonic terms in the potential.

The lowest levels observed but not predicted are \( 1^- \) and \( 3^- \) levels around 9 MeV. These levels might be accounted for if we assume that they belonged to the doubly degenerate E vibrational mode. But one would then have several other states in this region which are apparently not observed. Naturally, the \( 2^+; T=1 \) level at 10.27 MeV cannot be explained since the CAP model predicts only states with isotopic spin zero.

Besides the two doubly-degenerate E vibrations, the only normal mode not observed is the \( B^+_1 \) "twisting" vibration which describes the possible oscillation of the two dumbbells about the z axis. This mode is denoted \( \omega^3 \) in Table 2.11, and is characterized by a low-lying rotational spectrum of \( L=0^-, 2^-, 4^-, \ldots \). One can understand why this vibration is not observed by considering the hindered internal rotor of Figure 2.10b. If no potential barrier exists between the two dumbbells, the rotational Hamiltonian and wavefunction can be written as (17, pp. 491-500; 74, pp. 300-335)

\[
H_R = A_0 \left[ L(L+1) - \frac{1}{2} K^2 \right] + 2 A_3 m_1^2 + 2 A_3 m_2^2 \quad (2.111)
\]

and

\[
\langle \alpha \beta \gamma_1 \gamma_2 | L M; m_1, m_2 \rangle \sim e^{i L \alpha} d^L_m (B) e^{i m_1 \gamma_1} e^{i m_2 \gamma_2} \quad (2.112)
\]
In these equations, $m_1$ and $m_2$ are the angular momenta of each dumbbell about the body-fixed z axis, while the $2A_3$ of Equation 2.111 comes from the fact that the moment of inertia about the z axis of each dumbbell is half that of the total structure. By defining

$$\chi = \frac{\chi_1 + \chi_2}{2}, \quad \kappa = \frac{m_1 + m_2}{2}$$

$$\eta = \psi_2 - \psi_1, \quad \alpha = \frac{m_2 - m_1}{2}$$

(2.113)

one can rewrite Equations 2.111 and 2.112 as

$$H_R = A_1 \left( L (L+1) + K^2 (A_3 - A_1) \right) + 4 A_3 \alpha^2$$

(2.114)

and

$$\langle \alpha, \beta, \gamma, \eta | \sum \frac{1}{2} \psi_1 \psi_2 \rangle \sim e^{i M \alpha} d_{MK}^{LM} (\beta) e^{i \kappa \psi_1} e^{i \alpha \eta} D_{MK}^{L*} (\eta) e^{-i \eta}$$

(2.115)

where $\eta$ denotes the internal angle between the two dumbbells. The four angles $\eta, \gamma, \gamma_1, \gamma_2$ are defined in Figure 2.12. If the internal wavefunctions are to be single-valued, $m_1$ and $m_2$ must be integers. From Equation 2.113, we find that $K$ must then be integral and $\alpha$ half-integral. A further limitation on the quantum numbers arises from Bose-Einstein statistics, since the wavefunction of Equation 2.112 must now be invariant under $\gamma_1 \rightarrow \gamma_1 + \pi$ and $\gamma_2 \rightarrow \gamma_2 + \pi$. This additional restriction forces $m_1$ and $m_2$ to take on even integers or equivalently $K$ to be even and $\alpha$ to be integral.

In analogy to molecular calculations, we now introduce a suitable interaction between the two dumbbells and rewrite Equation 2.114 as

$$H_R = A_1 \left( L (L+1) + K^2 (A_3 - A_1) \right) - 4 A_3 \frac{\alpha^2}{\kappa^2} + V_0 \cos^2 \eta$$

(2.116)
Figure 2.12. Two different views of the $D_{2d}$ internal rotor. (a) Three dimensional view showing the four internal angles. The axes are labeled consistent with Figure 2.1. The alpha particles are numbered so that various permutation operations can be performed on the system. (b) Planar view of the same configuration looking down from the positive $Z'$ axis.
The last term has minima at $\eta = \pm 90^\circ$ and represents the potential barrier that each dumbbell must tunnel through in order for the structure to go from a right- to a left-handed system, and is shown in Figure 2.13. The wavefunctions are now of the form

$$\langle \Omega; \eta | L^{\nu} M K ; \mathbf{q} \rangle \sim \mathcal{D}_{M K}^{L \ast} (\Omega) \ M_{\mathbf{q}} (\eta) .$$

(2.117)

The $M_{\mathbf{q}} (\eta)$'s are related to Mathieu functions (74; p. 319) with the following limiting properties,

$$\lim_{V_0 \to 0} M_{\mathbf{q}} (\eta) \sim \cos (\sigma \eta) ; \sin (\sigma \eta)$$

(2.118)

$$\lim_{V_0 \to \infty} M_{\mathbf{q}} (\eta) \sim H_{\eta_3} (Q_3) ,$$

where $Q_3$ represents the "twisting" mode previously considered. The general shapes of the four lowest internal wavefunctions of interest are also drawn schematically in Figure 2.13.

The energy levels caused from the internal rotation can be readily found by diagonalizing the last two terms of Equation 2.116 among the free rotor wavefunctions of Equation 2.115. Instead of using the basis functions

$$\left\{ \frac{1}{\sqrt{\pi}} e^{i \sigma \eta} ; \sigma = 0, \pm 1, \pm 2, \cdots \right\} ,$$

we shall work with the alternate complete set,

$$\left\{ \sqrt{\frac{2}{\pi}} \cos (\sigma \eta) ; \sigma = 1, 2, 3, \cdots \right\}$$

(2.119)

and

$$\left\{ \sqrt{\frac{1}{\pi}} \sin (\sigma \eta) ; \sigma = 1, 2, 3, \cdots \right\} ,$$

(2.120)

since the matrix Hamiltonian will then conveniently separate into smaller spaces. This fact arises because the kinetic and potential terms of the internal rotation,
Figure 2.13. The shaded area represents the internal potential $V = V_0 \cos^2 \eta$. Also shown are schematics of the first four internal wavefunctions $M_n(\eta)$.

Table 2.12. The character table for the internal eigenfunctions $M_n(\eta)$ of the potential plotted in Figure 2.12.

<table>
<thead>
<tr>
<th>IR</th>
<th>$\eta \rightarrow \eta$</th>
<th>$\eta \rightarrow -\eta$</th>
<th>$\eta \rightarrow \pi + \eta$</th>
<th>$\eta \rightarrow \pi - \eta$</th>
<th>Basis function</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda_1$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>$M_1(\eta)$</td>
</tr>
<tr>
<td>$\lambda_2$</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>$M_2(\eta)$</td>
</tr>
<tr>
<td>$\lambda_3$</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>$M_3(\eta)$</td>
</tr>
<tr>
<td>$\lambda_4$</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>$M_4(\eta)$</td>
</tr>
</tbody>
</table>
\[ T = -4A_3 \frac{d^2}{d\eta^2} \]  
\( \) \hspace{1cm} (2.121)

and

\[ V = V_0 \cos^2 \eta \]  
\( \) \hspace{1cm} (2.122)

are symmetric in the transformation \( \eta \rightarrow -\eta \), and so matrix elements of the form \( \langle \cos(\sigma \eta) | T+V | \sin(\sigma \eta) \rangle \) are identically zero. The relevant matrix elements in the matrix Hamiltonian can be shown to be

\[
\frac{1}{2\pi} \langle \sin(\sigma' \eta) | T | \sin(\sigma \eta) \rangle = 4A_3 \sigma'^2 \delta_{\sigma \sigma'}
\]

\[
\frac{1}{2\pi} \langle \sin(\sigma' \eta) | V | \sin(\sigma \eta) \rangle = \frac{V_0}{4} \left\{ -\delta_{\sigma \eta} + 2\delta_{\sigma' \sigma' \eta} + \delta_{\sigma' \sigma' \eta} + \delta_{\sigma' \sigma' \eta} \right\}
\]

for the odd basis functions, and the following six for the even functions:

\[
\frac{1}{2\pi} \langle 1 | T | 1 \rangle = 0
\]

\[
\frac{1}{\sqrt{2}\pi} \langle 1 | T | \cos(\sigma \eta) \rangle = 0
\]

\[
\frac{1}{2\pi} \langle \cos(\sigma' \eta) | T | \cos(\sigma \eta) \rangle = 4A_3 \sigma'^2 \delta_{\sigma \sigma'}
\]

\[
\frac{1}{2\pi} \langle 1 | V | 1 \rangle = \frac{V_0}{2}
\]

\[
\frac{1}{\sqrt{2}\pi} \langle 1 | V | \cos(\sigma \eta) \rangle = \frac{\sqrt{2}}{4} V_0 \delta_{\sigma \eta}
\]

\[
\frac{1}{\pi} \langle \cos(\sigma' \eta) | V | \cos(\sigma \eta) \rangle = \frac{V_0}{4} \left\{ \delta_{\sigma \eta} + 2\delta_{\sigma' \sigma' \eta} + \delta_{\sigma' \sigma' \eta} + \delta_{\sigma' \sigma' \eta} \right\}
\]

From the explicit form of these elements, it is evident that additional symmetry is present in the Hamiltonian since all matrix elements between an even and an odd value of \( \sigma' \) are zero. This additional symmetry is, in fact, the invariance of the Hamiltonian under \( \eta \mapsto \eta + \pi \) and \( \eta \mapsto -\eta \). The basis functions \( M_{\frac{1}{2}}(\chi) \) then generate \( \mathbb{Z}_2 \)'s of a group isomorphic to \( \mathbb{Z}_2 \) as shown in
Table 2.12. Carrying out the diagonalization, one finds that the energy levels of the Hamiltonian in Equation 2.116 can be written as

$$E_{L,K_f} = A_1 (L+1) + K^2 (A_3 - A_1) + A_3 E_f \left( \frac{\nu_0}{A_3} \right), \quad (2.125)$$

where the last term is plotted in Figure 2.14. Notice that only certain $K^M$ bands can be built on each level. This restriction again arises from further application of Bose-Einstein statistics. From Figure 2.12, we see that the $D_{2d}$ symmetry no longer is present, but a group isomorphic to $D_{2d}$ elements exists; these elements can best be characterized by examining the way they permute the five particles of the rotor. For the time being we represent the basis functions of this group as

$$\Psi(\alpha, \beta, \gamma, \eta) \equiv \Psi_{LM}(\alpha, \beta, \gamma) M_z^{k}(\eta) \quad (2.126)$$

The eight permutation operations then act on this basis function as

$$(1)(2)(3)(4)(5) \Psi(\alpha, \beta, \gamma, \eta) = \Psi(\alpha, \beta, \gamma, \eta)$$

$$(12)(34)(5) \Psi(\alpha, \beta, \gamma, \eta) = \Psi(\alpha, \beta, \gamma + \eta, \eta)$$

$$(13)(24)(5) \Psi(\alpha, \beta, \gamma, \eta) = \Psi(\alpha + \eta, \beta - \gamma, \gamma, \eta)$$

$$(14)(23)(5) \Psi(\alpha, \beta, \gamma, \eta) = \Psi(\alpha + \eta, \beta - \gamma, \gamma - \eta, \eta)$$

$$(12)(34)(5) \Psi(\alpha, \beta, \gamma, \eta) = \Psi(\alpha - \eta, \beta + \gamma, \gamma, \eta - \eta)$$

$$(1)(2)(34)(5) \Psi(\alpha, \beta, \gamma, \eta) = \Psi(\alpha, \beta, \gamma + \frac{\eta}{2}, \eta + \eta)$$

$$(1324)(5) \Psi(\alpha, \beta, \gamma, \eta) = \Psi(\alpha + \eta, \beta - \gamma, \frac{\eta}{2} - \gamma, \eta + \eta)$$

$$(1423)(5) \Psi(\alpha, \beta, \gamma, \eta) = \Psi(\alpha + \eta, \beta - \gamma, \frac{\eta}{2} - \gamma, \eta - \eta) \quad (2.127)$$

By careful examination of these eight operations on the basis function of Equation 2.126, we find that wavefunctions symmetric under all eight operations are limited to those with $K^M$ bands, given in Figure 2.14. The parity
Figure 2.14. The part of the energy that depends on the internal rotation, $\mathcal{E}_t$, is plotted as a function of $V_0/A_3$. The correlation between torsional oscillation and free rotation is explicitly shown. The quantities $A_3$ and $V_0$ can be uniquely determined from the experimental positions of the first two $K=2$ bands. Bose statistics allow only certain $K^T$ bands to be built on each level.
of the wavefunction can now be carried out in a physical manner since the 
inversion operation is now equivalent to $C_{2x}$ followed by an internal rotat­
tion. One can then show that

$$I \Psi (\alpha, \beta, \gamma, \eta) = \Psi (\alpha + \alpha, \beta - \beta, \gamma - \gamma, -\eta).$$  \hspace{1cm} (2.128)$$

From Figure 2.14, it is also evident that for large $V_0/A_3$, the rotational 
approach those of the $D_{2d}$ rotor. The lower two internal levels degenerate 
into the zero-point vibrational mode with allowed $K^\pi$ bands of $0^+ (L \text{ even}),$ $2^-, 4^+, 6^-$, $\cdots$, and the next two will eventually degenerate into a one 
phonon mode of the twisting vibration with allowed bands of $K^\pi=0^- (L \text{ even}),$ $2^+, 4^-, 6^+$, $\cdots$. (See Table 2.1). Therefore, the parity of the $D_{2d}$ rotor 
wavefunction found physically by allowing for the tunneling procedure again 
corresponds to the results obtained from the mathematical formalism of Sec­
tion C.

By carefully examining Figure 2.14, we find that the inclusion of in­
ternal rotation thus alters only the $K^\pi$ bands of $\omega_3$, pulling the $K^\pi=2^+$ band 
far below the $0^-$ band for reasonable values of $V_0$. The value of $V_0$ could be 
estimated from the experimental separation energy of the $K=2^-$ and $K=2^+$ bands. 
Since no $L=3^+$ states are observed under 10 MeV, the $K=2^+$ band cannot start 
lower than the $L=2^+$ state at 9.5 MeV (c.f. Figure 2.11), and this fact im­
plies a separation energy of at least 4.5 MeV. By careful examination of 
Figure 2.14, we can then conclude that $V_0 > 10$ MeV and $0.7$ MeV $< A_3 < 1.0$ MeV. 
It should be noted that only two or three of the twenty states observed at 
present below 10 MeV are of unnatural parity. Thus it is conceivable that 
an $L=3^+$ state at approximately 8 MeV may be unobserved. If this were true, 
it would definitely lower our value for $V_0$. 
Unfortunately, no detailed electron scattering experiments have been performed for $^{20}$Ne. Such experiments would help determine the exact charge shape of the nucleus. For the $D_{2d}$ configuration, simple forms for the form factors (denoted $F_{L\kappa}^{\mp}$) may be found from Equations 2.56 and 2.58, and Figure 2.10a. These expressions for scattering to the lowest three levels are

$$F_{00}^{\mp} = \frac{1}{5} F_\alpha \left[ 1 + 4 \frac{j_0(q R_1)}{5} \right],$$

$$F_{20}^{\mp} = \frac{4/5}{F_\alpha} P_2(\cos \theta) \frac{j_2(q R_1)}{5},$$

and

$$F_{40}^{\mp} = \frac{12}{5} F_\alpha P_4(\cos \theta) \frac{j_4(q R_1)}{5}. \tag{2.129}$$

These same equations also hold for the hindered internal rotor of Figure 2.10b. In analogy with $^{28}$Si, for which the form factors have been measured, we expect the four outer alpha clusters to increase the radius of the inner one slightly. If this effect is included in our calculations, only the elastic form factor is changed, becoming

$$F_{00}^{\mp'} = \frac{1}{5} \left[ e^{-\frac{q^2 a_0^2}{6}} + 4 e^{-\frac{q^2 a^2}{6}} \frac{j_0(q R_1)}{5} \right], \tag{2.130}$$

where $a_0$ is the rms radius of the center alpha particle. The theoretical absolute squares of the form factors are plotted in Figure 2.15. From results on $^{28}$Si (which will be considered shortly), we choose $R_1$, $a_0$, and $a$ to be 2.65, 1.9, and 1.7 fm respectively for elastic scattering; but expect $R_1$ to increase to 3.0 fm for inelastic scattering because of centripetal distortion. We assume a reasonable value for $\theta$ of $30^\circ$. Of particular interest is the form factor for the $4^+$ level which is very sensitive to the choice of $\theta$. Indeed, the theoretical cross section $|F_{40}^{\pm}|^2$ increases by a factor of...
Figure 2.15. Theoretical cross sections for $^{20}\text{Ne}$: (a) elastic scattering form factors, (b) inelastic scattering form factors for the $2^+(1.63 \text{ MeV})$ and the $4^+(4.25 \text{ MeV})$ states. Solid line represents $a_0=1.9 \text{ fm}$, $a=1.7 \text{ fm}$, and $R_1=2.65 \text{ fm}$. From similar calculations on $^{28}\text{Si}$, we expect centripetal distortion to alter the parameters somewhat for the excited states. The dashed line represents the same parameters except $R_1=3.0 \text{ fm}$ and should give a better fit to the $L^=2^+$ state. In Figure 2.15b, $\Theta$ is taken to be $30^\circ$. 
10^2 if $\theta$ is changed by $\pm 5^\circ$ [since $P_4(\cos \theta)$ goes through one of its zeros at $=30.6^\circ$]. With $R_1=2.65$ fm and $\theta=30^\circ$, the intrinsic electric moments are calculated to be $Q_{20}=70.2$ fm$^2$ and $|E_{32}|=|E_{3,-2}|=44.2$ fm$^3$. With $\theta=25^\circ$, the results change to $Q_{20}=81.9$ fm$^2$ and $|E_{32}|=|E_{3,-2}|=32.9$ fm$^3$. The quadrupole moments compare favorably with Table 2.10.

Table 2.13 compares experimental transitions of low-lying states with those predicted by the structure. The values for the two parameters are taken to be $|Q_{20}|=58.3$ fm$^2$ and $|E_{32}|=|E_{3,-2}|=27.3$ fm$^3$ which are fairly close to those indicated in the previous paragraph.

4. \textit{24}Mg and the asymmetric rotor

The $\alpha$-structure usually assumed for \textit{24}Mg is the D$_{4h}$ square bipyramid shown in Figure 2.16a. All low-lying levels can be accounted for if one assumes the $K^\pi=2^+$ band beginning at 4.23 MeV is built on a normal vibration belonging to the $B_{1g}$ IR of D$_{4h}$ (c.f. Table 2.1). However, a low-lying \textit{K}$^\pi=0^+$ band is predicted but not observed at around 4 MeV (22). Also, this configuration gives a poor fit to the electron scattering data and predicts a negative intrinsic quadrupole moment (35) contrary to the results given in Table 2.10.

Reviewing the other possible configurations, we find that a structure with D$_{2h}$ symmetry, which has not been considered before, will also account for the same energy levels, and further with one less parameter. Also, the $K^\pi=2^+$ band is not then built on a vibration, and one can give explicit expressions for the electron scattering form factors of these states as was not done in the D$_{4h}$ case. There are two possible nonplanar structures with this symmetry (Figure 2.16b,c). Although both structures predict the same
Table 2.13. Comparison of theoretical and experimental values for certain transitions in $^{20}$Ne. The values for the two parameters are $|q_{20}| = 58.3 \text{ fm}^2$ and $|E_{32}| = 27.3 \text{ fm}^2$.

| Initial State ($L^+ - \text{MeV}$) | Final State ($L^+ - \text{MeV}$) | Type of Transition | Transition Rate (in terms of Weisskopf units - $|M|^2$) |
|-----------------------------------|---------------------------------|-------------------|---------------------------------|
| $2^+ - 1.63$                      | $0^+ - 0.0$                     | E2                | Experiment: $24.2 \pm 2.5$ $^a$  |
|                                   |                                 |                   | Theory: 21.0                     |
| $4^+ - 4.25$                      | $2^+ - 1.63$                    | E2                | Experiment: $16.2 \pm 2.8$ $^a$ |
|                                   |                                 |                   | Theory: 30.0                     |
| $6^+ - 8.79$                      | $4^+ - 4.25$                    | E2                | Experiment: $28.0 \pm 6.0$ $^a$  |
|                                   |                                 |                   | Theory: 33.0                     |
| $8^+ - 11.99$                     | $6^+ - 8.79$                    | E2                | Experiment: $-$                   |
|                                   |                                 |                   | Theory: 34.6                     |
| $2^- - 4.97$                      | $0^+ - 0.0$                     | E2                | Experiment: $0.002$ $^b$         |
|                                   |                                 |                   | Theory: 0.0                       |
|                                   | $2^+ - 1.63$                    | E1                | Experiment: $7.4_{-1.9}^{+2.1} \times 10^{-6}$ $^c$ |
|                                   |                                 |                   | Theory: 0.0                       |
|                                   | $0^+ - 0.0$                     | M2                | Experiment: $0.017$ $^b$          |
|                                   |                                 |                   | Theory: 0.0                       |
|                                   | $2^+ - 1.63$                    | E3                | Experiment: $5.8_{-3.5}^{+5.1}$ $^b$ |
|                                   |                                 |                   | Theory: 12.5                      |
| $3^- - 5.63$                      | $0^+ - 0.0$                     | E3                | Experiment: $7_{-2}^{+3}$ $^b$    |
|                                   |                                 |                   | Theory: 5.0                       |
|                                   | $2^+ - 1.63$                    | E1                | Experiment: $4.1_{-0.8}^{+1.3} \times 10^{-6}$ $^c$ |
|                                   |                                 |                   | Theory: 0.0                       |
|                                   | $0^+ - 0.0$                     | M2                | Experiment: $-$                   |
|                                   |                                 |                   | Theory: 0.0                       |
|                                   | $2^+ - 1.63$                    | E3                | Experiment: $<3.0$ $^b$           |
|                                   |                                 |                   | Theory: 0.0                       |
| $4^- - 7.02$                      | $2^+ - 1.63$                    | M2                | Experiment: $\leq 0.14$ $^b$      |
|                                   |                                 |                   | Theory: 0.0                       |
|                                   | $2^+ - 1.63$                    | E3                | Experiment: $\leq 6.0$ $^b$       |
|                                   |                                 |                   | Theory: 6.7                       |


$^b$Broude et al., Can. J. Phys. 45, 1837 (1967). (75)

$^c$Evans et al., Can. J. Phys. 45, 82 (1967). (76)
Figure 2.16. Some of the possible structures for $^{24}\text{Mg}$, along with the parameters that can be varied to fit experimental data.
energy spectrum, the bitetrahedron (Figure 2.16c) is found to be in better agreement with the experimental electron scattering form factors and so should be the correct structure. Other possible configurations have been eliminated previously (24). The calculation of the energy levels for this structure is like that for the asymmetric rotor of Davydov and Fillipov in (41, pp. 292-301), since both models have the same spatial symmetry ($D_{2h}$). In fact, the existence of this particular $\alpha$-structure might explain why the asymmetric rotor works well in $^{24}$Mg, but not for $^{20}$Ne or $^{28}$Si.

Table 2.1 lists the rotational quantum numbers for each IR of $D_{2h}$. Since a $D_{2h}$ structure constitutes an asymmetric rotor, the energies must be found by diagonalizing the Hamiltonian in Equation 2.11 among all rotational wavefunctions of the same L and same $D_{2h}$ symmetry. For the pure rotational spectrum, it proved more convenient to vary three new parameters uniquely determined by the $A_J$. These parameters are the rotational energies of the first two $L=2^+$ states (denoted $E_2$ and $E_2'$) and a parameter $\gamma$ which determines the wavefunctions of these two states in the form

$$<\alpha|2^+_M> = \frac{5}{\sqrt{8\pi^2}} \left\{ \cos \gamma D^2_{M0} (\alpha) + \frac{1}{2} \sin \gamma \left[ D^2_{M2} (\alpha) + D^2_{M-2} (\alpha) \right] \right\}$$

$$<\alpha|2^{'+}_M> = \frac{5}{\sqrt{8\pi^2}} \left\{ -\sin \gamma D^2_{M0} (\alpha) + \frac{1}{2} \cos \gamma \left[ D^2_{M2} (\alpha) + D^2_{M-2} (\alpha) \right] \right\}$$

The dependence of these three parameters on the rotational parameters, $A_K$, can be found by constructing the 2x2 energy matrix for the $L=2^+$ levels and solving for the eigenvalues analytically. The resultant three relations can most easily be expressed as

$$A_1 + A_2 + A_3 = \frac{1}{4} \left( E_2 + E_2' \right)$$
\[ 2A_3^2 - A_1^2 - A_2^2 = \frac{1}{2} \cos(2\gamma)(E_{2'} - E_2) \] (2.132)

\[ \sqrt{3}(A_2 - A_1) = \frac{1}{2} \sin(2\gamma)(E_{2'} - E_2) \]

Figure 2.17 is a graph of the rotational energies built on the zero-point vibrational state. Both \( E_2 \) and \( E_{2'} \) are fixed by experiment, and \( \gamma \) is allowed to vary between \( \pm 90^\circ \). The periodicity of the levels in \( \gamma \) shows that these energies are symmetric under the six permutations of the \( A_i \). Only those experimental levels of \(^{24}\text{Mg}\) associated with the zero-point vibrational mode are shown. Good results are obtained only for the redundant values \( \gamma = 0^\circ, \pm 60^\circ \); consequently \(^{24}\text{Mg}\) is very nearly a prolate symmetric top as assumed in Table 2.10. Figure 2.16c is drawn with \( \gamma \leq 10^\circ \).

The rotation-vibration interactions were found to affect the energy levels just enough to make it virtually impossible to determine \( \gamma \) more accurately than already given. Thus, for simplicity, we set \( \gamma = 0^\circ \) and calculate the energy levels of \(^{24}\text{Mg}\) using the symmetric top formula of Equation 2.6. Figure 2.18 shows the best correlation of theoretical levels with experiment. The experimental levels are taken from References (67) and (77). The twelve possible normal vibrations allowed by the structure are given in Table 2.14. Again, the lower limits assigned to some of the rotational parameters cause the pertinent excited states to lie above 10 MeV. An excitation of a normal vibration may cause the rotor to become highly asymmetric, making the band structure of the states between 7 and 10 MeV less apparent than in \(^{20}\text{Ne}\). The only observed state below 9 MeV that is uncorrelated with theory is an \( K^P = 3^- \) level at 7.02 MeV.
Figure 2.17. Variation of theoretical energy levels of the asymmetric rotor as a function of the asymmetry parameter $\gamma$. Note that good agreement with the experimental spectrum is obtained only for $\gamma \leq 0^\circ$, $\pm 60^\circ$. Inclusion of centripetal distortion would lower theoretical levels of high spin, and would give even better agreement with experiment.
Figure 2.18. Comparison of experimental levels of $^{24}\text{Mg}$ with the theoretical levels predicted from the $D_{2h}$ bitetrahedron. The energy scale is again changed at 7 MeV. The bitetrahedron can also be viewed as a $D_{2h}$ rectangular bipyramid with the rectangle in the plane of the paper.
Table 2.14. Possible normal vibrations for the $D_{2h}$ bitetrahedron structure of $^{24}\text{Mg}$.

<table>
<thead>
<tr>
<th>Frequency</th>
<th>$\omega_1$</th>
<th>$\omega_2$</th>
<th>$\omega_3$</th>
<th>$\omega_4$</th>
<th>$\omega_5$</th>
<th>$\omega_6$</th>
<th>$\omega_7$</th>
<th>$\omega_8$</th>
<th>$\omega_9$</th>
<th>$\omega_{10}$</th>
<th>$\omega_{11}$</th>
<th>$\omega_{12}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Irreducible Representation</td>
<td>$A_g$</td>
<td>$A_g$</td>
<td>$A_g$</td>
<td>$A_u$</td>
<td>$B_1g$</td>
<td>$B_{1u}$</td>
<td>$B_{1u}$</td>
<td>$B_{2g}$</td>
<td>$B_{2u}$</td>
<td>$B_{2u}$</td>
<td>$B_{3g}$</td>
<td>$B_{3u}$</td>
</tr>
<tr>
<td>Observed Energy of Excitation (MeV)</td>
<td>0.0</td>
<td>6.5</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>7.6</td>
<td>7.3</td>
<td>8.2</td>
<td>$\approx$9.2</td>
<td>$\approx$8.6</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

$A_1 = A_2$ | 0.18 | 0.10 | - | - | - | 0.10 | 0.10 | 0.10 | $\approx$0.10 | $\approx$0.10 | - | - | - |

Rotational parameters (MeV) $A_3$ | 0.90 | 0.55 | - | - | - | $\geq$0.55 | $\geq$0.63 | $\geq$0.40 | $\approx$0.50 | $\approx$0.50 | - | - | - |
From Equations 2.68 and 2.131, we can relate the intrinsic electric quadrupole moments to certain observed quantities. The pertinent equations are

\[
\begin{align*}
\sqrt{2} Q_{22} \sin 2\gamma - Q_{20} \cos 2\gamma &= \frac{2}{5} \sqrt{4\pi} \left< 2^+ \| E(2) \| 2^+ \right> = -87 \pm 12 \text{ fm}^2, \\
\sqrt{2} Q_{22} \sin \gamma + Q_{20} \cos \gamma &= 2 \sqrt{\frac{4\pi}{5}} \left< 0^+ \| E(2) \| 2^+ \right> = \pm 78 \pm 9 \text{ fm}^2, \\
\sqrt{2} Q_{22} \cos 2\gamma + Q_{20} \sin 2\gamma &= \frac{2}{5} \sqrt{4\pi} \left< 2^+ \| E(2) \| 2^+ \right> = \pm 19 \pm 3 \text{ fm}^2, \\
\sqrt{2} Q_{22} \cos \gamma - Q_{20} \sin \gamma &= 2 \sqrt{\frac{4\pi}{5}} \left< 0^+ \| E(2) \| 2^+ \right> = \pm 15 \pm 3 \text{ fm}^2, \\
\end{align*}
\]

and

\[
\sqrt{2} Q_{22} \cos \gamma - Q_{20} \sin \gamma = \frac{4}{5} \sqrt{\frac{4\pi}{5}} \left< 3^+ \| E(2) \| 2^+ \right> = \pm 23^{+16}_{-6} \text{ fm}^2,
\]

where the experimental values are taken from Table 2.10 and Reference (78).

A careful examination of these equations together with \(|\gamma| \leq 10^\circ\) shows that

\[Q_{20} = 75 \pm 10 \text{ fm}^2,\]

and

\[|Q_{22}| \leq 15 \text{ fm}^2.\]  \hspace{1cm}(2.134)

The only magnetic transition that has been measured among the states of the ground state rotational band of {superscript 24}Mg is an M1 transition between the {superscript 2}+(4.23 MeV) and {superscript 2}+(1.37 MeV) states. Its value in terms of Weisskopf units is (78)

\[|M^2|_{\text{w.u.}} = 6^{+17}_{-4} \times 10^{-6},\]  \hspace{1cm}(2.135)

which is in good agreement with the zero-value predicted by all collective models.

With \(\gamma=0^\circ\), the electron scattering form factors for {superscript 24}Mg are found from Equations 2.56, 2.58, and Figure 2.16c. These equations are
\[ F_{00}^+ = \frac{1}{3} F_\alpha \left[ \frac{1}{2} (\mathbf{q} \cdot \mathbf{r}_1) + 2 \frac{1}{2} (\mathbf{q} \cdot \mathbf{r}_2) \right] , \]
\[ F_{20}^+ = \frac{\sqrt{5}}{6} F_\alpha \left[ -\frac{1}{2} (\mathbf{q} \cdot \mathbf{r}_1) + 4 \frac{1}{2} \cos \theta \frac{1}{2} (\mathbf{q} \cdot \mathbf{r}_2) \right] , \]
\[ F_{40}^+ = F_\alpha \left[ \frac{3}{8} \frac{1}{2} (\mathbf{q} \cdot \mathbf{r}_1) + 2 \frac{1}{2} \cos \theta \frac{1}{2} (\mathbf{q} \cdot \mathbf{r}_2) \right] , \]
\[ F_{22}^+ = \frac{\sqrt{5}}{6} F_\alpha \left[ \frac{1}{2} (\mathbf{q} \cdot \mathbf{r}_1) - 2 \sin^2 \theta \frac{1}{2} (\mathbf{q} \cdot \mathbf{r}_2) \right], \quad (2.136) \]
\[ F_{32}^+ = 0 \]

and
\[ F_{42}^+ = -\frac{\sqrt{5}}{4} F_\alpha \left[ \frac{1}{2} (\mathbf{q} \cdot \mathbf{r}_1) + 2 \sin \theta \cos \theta (\mathbf{q} \cdot \mathbf{r}_2) \right] , \]

where \( R_1, R_2, \) and \( \theta \) are defined in Figure 2.16c.

We first vary \( R_1, R_2, \) and \( a \) to agree with the elastic scattering data. The best fit is \( R_1=1.7 \text{ fm}, R_2=2.7 \text{ fm}, \) and \( a=1.9 \text{ fm} \) as shown in Figure 2.19a. These parameters are identical to the previous \( D_{4h} \) ones (35) since the two structures have the same theoretical elastic form factor. Other sets of parameters were also found which gave nearly as good results. We now vary \( \theta \) to fit the inelastic curve for the \( 2^+ \) state at 1.37 MeV. The best value is \( \theta=30^\circ \) which yields the solid line in Figure 2.19b. Theoretical curves for the cross sections of the two higher states (solid lines in Figures 2.19c and 2.19d) are not entirely reproduced by this set of parameters. Unfortunately, the \( 4^+(4.12 \text{ MeV}) \) and \( 2^+(4.23 \text{ MeV}) \) states appear as an experimental unresolved doublet, so the theoretical cross sections of these two levels must be added. As expected, scattering to the \( 3^+ \) state at 5.22 MeV was not experimentally observed.

The results can be improved somewhat if we also vary the asymmetry parameter \( \gamma \). Since we now have an asymmetric rotor, the cross sections cannot
Figure 2.19. Experimental and theoretical form factors for the $D_{2h}$ bitetrahedron of $^{24}$Mg: (a) elastic scattering form factor; (b), (c), (d) various inelastic scattering form factors. Centripetal distortion, which has the effect of compressing the theoretical curves towards the ordinate axis (as shown in Figures 2.15 and 2.22), was not considered because of the number of parameters already used. Inclusion of this effect would definitely give better results for Figures 2.19c and 2.19d.
be found in simple forms, but are still computed from Equations 2.56 and 2.58. Here is where we make use of the fact that the \( a_{NK}^L \) depend upon only one parameter, which in this case is \( \gamma \). Like \( \theta \), this parameter has no effect on the elastic scattering cross section of Figure 2.19a. The dashed lines in Figures 2.19c and 2.19d represent the same parameters as before, except that the asymmetry parameter is now \( \gamma = +10^\circ \). The form factor for the \( 2^+(1.37 \text{ MeV}) \) level is only slightly altered by this change in \( \gamma \) and is not shown in Figure 2.19b. Since \( R_1, R_2, \theta, \) and \( \gamma \) have now been determined, we can calculate the intrinsic quadrupole moments, which are \( Q_{20} = 61.2 \text{ fm}^2 \) and \( Q_{22} = -3.7 \text{ fm}^2 \), close to the values given in Equation 2.134. Reasonable values of the five parameters \( (R_1, R_2, a, \theta, \text{ and } \gamma) \) have thus led to four good cross-section curves. In addition, these same parameters correctly predict several reduced matrix elements.

5. **An oblate structure for \( ^{28}\text{Si} \)**

Looking at the experimental spectrum (67,79) of \( ^{28}\text{Si} \) (Figure 2.20), we find that the lowest three levels indicate some form of collective rotation. However, these levels do not follow the \( L(L+1) \) rule as well as the corresponding levels in \( ^{20}\text{Ne} \) and \( ^{24}\text{Mg} \). There also appear to be \( K=3^+ \) and \( K=3^- \) bands starting at 6.27 and 6.88 MeV respectively. The \( D_{3d} \) bitetrahedron (Figure 2.21a), which was considered to be the best structure in a previous paper (23), can account for both bands if one allows for the possibility of internal rotation between the two triangular clusters. The calculations are very similar to those already done for the \( D_{2d} \) hindered rotor in \( ^{20}\text{Ne} \), the small energy separation between the two \( K=3 \) bands implying that this structure has nearly free internal rotation. The symmetry group that arises is
Figure 2.20. Comparison of the experimental levels of $^{28}\text{Si}$ with the theoretical levels predicted from the oblate $D_{3d}$ structure. The energy scale is again changed at 7 MeV.
Figure 2.21. Some of the possible configurations for $^{28}\text{Si}$.
unlike the $^{20}\text{Ne}$ case (c.f. Table 2.12) in that it is not isomorphic to any standard point group. Nevertheless, such a finite group has been developed in the literature (80), because many molecules (such as $\text{C}_2\text{H}_6$ and $\text{C}_2\text{D}_6$) have this symmetry. Unfortunately, recent experiments that measure the static quadrupole moment of the $2^+(1.78 \text{ MeV})$ state show that $^{28}\text{Si}$ is oblate, a fact definitely eliminating Figure 2.21a as a possible structure. An oblate $D_{3d}$ structure as shown in Figure 2.21b leads to only the $K=3^+$ band. Similarly, the oblate $D_{3h}$ structure of Figure 2.21c predicts only the $K=3^-$ band. The $D_{5h}$ bipyramid (Figure 2.21d), which is the usual configuration considered for $^{28}\text{Si}$, predicts only $K=1^+, 2^+, \text{ or } 5^+$ bands in this region (c.f. Table 2.1). A planar $D_{6h}$ hexagon with one alpha cluster in the center can account for both $K=3$ bands by assuming they are built on separate normal vibrations. However, this structure is unlikely; it leads to a negative intrinsic quadrupole moment twice as large as experiment. Other configurations besides those already mentioned were considered in Reference (23) and discarded.

Of the configurations that have the proper quadrupole moment, the one that predicts the most low-lying energy levels is the oblate $D_{3d}$ structure of Figure 2.21b. The $K^*$ bands allowed for each IR of $D_{3d}$ are given in Table 2.1, and the possible normal vibrations are listed in Table 2.15 along with values for the excitation energies of observed normal vibrations. Again, in order to push certain states above 10 MeV, lower limits are given to several of the rotational parameters. The results are not as good as for the previous two nuclei. A low-lying $L^*=2^+$ state is predicted at approximately 6.2 MeV which is not observed (Figure 2.20). However, this state would also be
Table 2.15. Possible normal vibrations for the oblate D₃d structure of ²⁸Si.

<table>
<thead>
<tr>
<th>Frequency</th>
<th>ω₁</th>
<th>ω₂</th>
<th>ω₃</th>
<th>ω₄</th>
<th>ω₅</th>
<th>ω₆</th>
<th>ω₇</th>
<th>ω₈</th>
<th>ω₉</th>
<th>ω₁₀</th>
</tr>
</thead>
<tbody>
<tr>
<td>Irreducible Representation</td>
<td>A₁g</td>
<td>A₁g</td>
<td>A₁g</td>
<td>A₁u</td>
<td>A₂u</td>
<td>A₂u</td>
<td>Eᵣ</td>
<td>Eᵣ</td>
<td>Eᵣ</td>
<td>Eᵣ</td>
</tr>
<tr>
<td>Observed Energy of Excitation (MeV)</td>
<td>0</td>
<td>5.0</td>
<td>6.7</td>
<td>~7.9</td>
<td>~8.0</td>
<td>6.7</td>
<td>~8.2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Rotational Parameters (MeV)</td>
<td>A₁ = A₂</td>
<td>0.20</td>
<td>0.20</td>
<td>0.15</td>
<td>~0.18</td>
<td>~0.17</td>
<td>0.12</td>
<td></td>
<td>0.12</td>
<td></td>
</tr>
<tr>
<td></td>
<td>A₃</td>
<td>0.55</td>
<td>≥0.49</td>
<td>≥0.32</td>
<td>~0.60</td>
<td></td>
<td></td>
<td></td>
<td>~0.6</td>
<td></td>
</tr>
</tbody>
</table>
predicted by all other symmetric top configurations. As in \( ^{24}\text{Mg} \), the lowest state observed but not predicted is a \( 3^- \) state at 6.88 MeV.

The theoretical form factors for the low-lying \( K^Z = 0^+ \) states of this structure are

\[
F_{00}^+ = \frac{i}{7} F_\alpha [1 + 6 \hat{\phi}_0(qR_i)]
\]

\[
F_{20}^+ = \frac{6}{7} \sqrt{3} F_\alpha P_2(\cos \Theta) \hat{\phi}_2(qR_i)
\]

and

\[
F_{40}^+ = \frac{18}{7} F_\alpha P_4(\cos \Theta) \hat{\phi}_4(qR_i)
\]

(2.137)

Comparing these equations with experiments, taken from Reference (35), one finds that the elastic scattering form factor can only be well predicted if one assumes that the central alpha particle is slightly larger than the other six. In this case, only the elastic form factor changes, becoming

\[
F_{00}' = \frac{i}{7} [e^{-g^2a_0^2/6} + 6 \hat{\phi}_0(qR_i)e^{-g^2a_0^2/6}]
\]

(2.138)

Since these formulae are independent of the azimuthal angle of the alpha clusters, they also apply to the oblate \( D_{3h} \) structure of Figure 2.21c.

The experimental elastic scattering curve can now be reproduced very well with several different sets of parameters (Figure 2.22a). However, all of them predict the parameter \( a_0 \) to be about 0.2 fm larger than \( a \). The angle \( \Theta \) can then be varied to fit the \( 2^+(1.78 \text{ MeV}) \) curve. The solid line in Figure 2.22 represents the best fit with \( a_0 = 1.9 \text{ fm} \), \( a = 1.7 \text{ fm} \), \( R_1 = 2.65 \text{ fm} \), and \( \Theta = 63^\circ \). The theoretical form factor for the \( 2^+ \) state can be improved if one allows for centripetal distortion by increasing \( R_1 \). This improvement is shown in Figure 2.22b by the dashed curve which is drawn for \( a_0 = 1.9 \text{ fm} \), \( a = 1.7 \text{ fm} \), \( R_1 = 3.0 \text{ fm} \), and \( \Theta = 64^\circ \). Naturally, one expects these new parameters
Figure 2.22. Experimental and theoretical form factors for $^{28}\text{Si}$: (a) elastic scattering form factors, (b) inelastic scattering form factors for 1.78 MeV $2^+$ state ($\dagger$), and the 4.61 MeV $4^+$ state ($\ddagger$).
to give a poorer fit for the elastic curve. Using $R_1 = 3.0$ fm and $\Theta = 64^\circ$, the intrinsic quadrupole moment is found to be $Q_{20} = -45.8$ fm$^2$ which compares favorably with the value obtained from the measured $2^+$ static quadrupole moment of Table 2.10, as well as with the moment determined from various transitions (Table 2.16).

A similar calculation (35) of the form factors has been done for $^{28}\text{Si}$ with the $D_{5h}$ pentagonal bipyramid of Figure 2.21d. As in the $D_{3d}$ case, new values for the parameters were needed to fit the inelastic scattering curves. Although the resultant theoretical curves are equally as good as those given in Figure 2.22, the parameters for inelastic scattering needed to be changed in the opposite direction from that which one would expect for centripetal distortion. Since the $D_{3d}$ structure also predicts most of the observed low-lying levels, it should be preferred over the $D_{5h}$ bipyramid.

6. **The inconclusive results of $^{32}\text{S}$ and $^{36}\text{Ar}$**

It is interesting to note that the experimental energy spectra (67,71) of both $^{32}\text{S}$ and $^{36}\text{Ar}$ (Figures 2.23 and 2.24) have $0^+$, $2^+$, $4^+$, and $3^-$ levels at approximately twice the energy of the first $2^+$ state in good agreement with the collective vibrator model (c.f. Section 111B). Moreover, no definite $K^\pi$ bands other than possibly the ground state $0^+$ band are observed in either nucleus. Also, from the last column of Table 2.10, it appears that the low-lying states of $^{32}\text{S}$ are not of the same character as those of $^{20}\text{Ne}$, $^{24}\text{Mg}$, and $^{28}\text{Si}$. As a consequence, one does not expect the CAP model to work as well here as for the nuclei previously considered.

Most of the possible structures for $^{32}\text{S}$ appear in Reference (23), where it was concluded that this nucleus most likely had $D_{3d}$ or $D_{3h}$ symmetry.
Table 2.16. Comparison of theoretical and experimental values for certain transitions in $^{28}$Si using the $D_{3d}$ structure. The single parameter is taken to be $|Q_{20}| = 50.2 \text{ fm}^2$.

| Initial State ($L^\pi - \text{MeV}$) | Final State ($L^\pi - \text{MeV}$) | Type of Transition | TRANSITION RATE (in terms of Weisskopf units $-|M^2|$) |
|-------------------------------------|------------------------------------|--------------------|----------------------------------------------------|
|                                     |                                    |                    | Experiment                                         |
|                                     |                                    |                    | Theory                                             |
| $2^+ - 1.78$                       | $0^+ - 0.0$                        | E2                 | $14.7 \pm 1.6^a$                                   |
|                                    |                                    |                    |                                                    | $10.0$ |
| $4^+ - 4.61$                       | $2^+ - 1.78$                       | E2                 | $9.5 \pm 2.2^a$                                    |
|                                    |                                    |                    |                                                    | $14.3$ |
| $6^+ - 8.54$                       | $4^+ - 4.61$                       | E2                 | $9.4 \pm 3.0^a$                                    |
|                                    |                                    |                    |                                                    | $15.7$ |
| $3^+ - 6.27$                       | $2^+ - 1.78$                       | E2                 | $0.001^b$                                          |
|                                    |                                    |                    |                                                    | $0.0$  |
| $4^+ - 6.89$                       | $2^+ - 1.78$                       | E2                 | $1.1 \pm 0.2^b$                                    |
|                                    |                                    |                    |                                                    | $0.0$  |
| $3^- - 6.88$                       | $0^+ - 0.0$                        | E3                 | $18.0 \pm 13.0^b$                                  |
|                                    |                                    |                    |                                                    | -      |


Figure 2.23. Comparison of experimental levels of $^{32}$S with theory predicted from two different structures. Also shown are the IR's for the observed normal modes. The parameters used (in MeV) are: (a) $D_{2h}$ structure: $A_1 = A_2 = 0.25$, $A_3 = 0.90$, $\hbar \omega_1 = 3.8$, $\hbar \omega_2 = 4.0$, and $\hbar \omega_3 = 4.4$. (b) $D_{3h}$ structure: $A_1 = A_2 = 0.20$, $A_3 = 0.50$, $\hbar \omega_1 = 3.5$, $\hbar \omega_2 = 4.0$, and $\hbar \omega_3 = 5.4$. 
Figure 2.24. Comparison of experimental levels of $^{36}$Ar with theory predicted by two different structures. The IR's for observed normal modes are also shown. In both structures, the vibration that contains two quanta of $\hbar \omega_2$ occurs at relatively low energy and is denoted $\hbar \omega_3$. The parameters used (in MeV) are: (a) $D_{4d}$ structure: $A_1=A_2=0.20$, $A_3=0.32$, $\hbar \omega_1=4.0$, $\hbar \omega_2=3.0$, and $\hbar \omega_3=5.4 \pm 2 \hbar \omega_2$. (b) $D_{5d}$ structure: $A_1=A_2=0.20$, $A_3=0.17$, $\hbar \omega_1=4.0$, $\hbar \omega_2=3.1$, $\hbar \omega_3=5.4 \pm 2 \hbar \omega_2$. 
Reviewing the calculations with more recent and extensive experimental data, we find that $D_{3h}$ and $D_{2h}$ structures (Figure 2.25) give reasonable fits, with a $D_{3d}$ structure not completely ruled out. Results for the $D_{2h}$ and $D_{3h}$ structures are plotted in Figure 2.23, together with the experimental data. Unlike our calculations for the previous nuclei, the same set of rotational parameters is used over all normal vibrations. Again, for both structures, the first level observed but not predicted is of spin $L=3$ at around 5 MeV.

Structures of higher symmetry (such as the $D_{6d}$ hexagonal bipyramid, Figure 2.25b, the $D_{7h}$ body-centered planar heptagon, etc.) can account for all low-lying levels if one introduces five or six normal vibrations. However, these structures predict an oblate shape contrary to experiment, and introduce too many parameters to be really meaningful.

The nucleus $^{36}$Ar is similar to $^{20}$Ne and $^{28}$Si in that it contains an odd number of alpha clusters. Since both $^{20}$Ne and $^{28}$Si were found to have an alpha particle in the center, one of the most likely candidates for $^{36}$Ar is the $D_{4d}$ body-centered square antiprism of Figure 2.25c. Another possibility is the $D_{5h}$ planar pentagon where four of the alpha clusters form an $^{16}$O core (Figure 2.25d). Both of these structures give fair agreement with experiment as is shown in Figure 2.24. The first level observed but not predicted is an $L=3^-$ level at 4.18 MeV. Again, configurations of higher symmetry can account for all levels if enough parameters are introduced, but such agreement is not very satisfying.

It should be noted that both structures given for $^{36}$Ar have double vibrations (denoted $\hbar\omega_3$ in Figures 2.24a and 2.24b) which occur at relatively low energy. Unlike the corresponding $\omega_2^*$ double vibration of $^{20}$Ne, both of these modes contain two quanta of a doubly-degenerate vibration. The
Figure 2.25. Two possible configurations each for $^{32}\text{S}$ (Figures a and b), and $^{36}\text{Ar}$ (Figures c and d).
allowed IR's for these modes are thus found by taking the appropriate symmetric direct product (30, pp. 132-134). All antisymmetric wavefunctions of the direct product will identically vanish.

7. The $O_h$ symmetry of $^{40}$Ca

Unlike all other nuclei considered in this paper, $^{40}$Ca does not have $L=2^+$ for its first excited state (c.f. Figure 2.25a). Consequently, $^{40}$Ca has no permanent quadrupole deformation in its ground state and the momental ellipsoid of any $\alpha$-structure for this nucleus must be that of a spherical top (i.e. $A_1=A_2=A_3$). The only reasonable configuration satisfying these conditions is the structure shown in Figure 2.26b. It consists of six alpha clusters arranged in an octahedron outside of four others which form a tetrahedral $^{16}$O core. The similarity of this structure with the corresponding shell model description is especially appealing.

The low-lying excited states of this structure should be very complicated because one now has ten particles to contend with, and also because Coriolis forces are known to be extremely important in spherical top configurations (19,20). Indeed, there is even reason to believe that some of the excited states, such as the first excited $0^+$, $2^+$, and $4^+$ levels, may be built on permanently deformed rotational bands. A similar situation was shown previously to exist in $^{16}$O. As a first approximation, one could assume that the $^{16}$O core does not contribute to the overall rotation of the nucleus. The structure would then have $O_h$ symmetry, and the first three negative parity states could be qualitatively explained as rotational states built on a normal vibration of the $F_{1u}$ IR, which contains levels of spin $L=3^-$, $4^-$, $5^-$, $6^-$, $\cdots$ (30, p. 333). Because of the complexity of the
Figure 2.26. Some general information on $^{40}$Ca. (a) Experimental energy levels of $^{40}$Ca. (b) Most realistic structure for $^{40}$Ca is an octahedron outside of a tetrahedral $^{16}$O core. (c) Comparison of experimental elastic electron form factor with that predicted by the structure in (b).
problem, no attempt was made to calculate the level spectrum explicitly, however.

From recent experiments (82,83), the absolute form factor \( |F_{00}^+| \) for elastic electron scattering on \(^{40}\text{Ca}\) is known very well, and is shown as the dotted curve in Figure 2.26c. This curve was obtained indirectly in References (82) and (83) by first fitting a phenomenological charge distribution of six parameters to experimental differential cross-sections, using partial-wave analysis, and then calculating \(|F_{00}^+|\) by taking the Fourier transform of this charge distribution. Because of the method used, no error bars were drawn for this curve, but they should be quite small except for possibly \( q > 3 \text{ fm}^{-1} \). All present experiments give points between \( 0.7 \text{ fm}^{-1} \leq q \leq 3.2 \text{ fm}^{-1} \).

The theoretical form factor is obtained directly from Equations 2.56, 2.58, and Figure 2.26b as

\[
|F_{00}^+| = \frac{1}{10} e^{-8^2\alpha^2/6} \left[ 4 \hat{f}_0(qR_1) + 6 \hat{f}_0(qR_2) \right],
\]

(2.139)

where \( R_1 \) and \( R_2 \) are the radial distances to the alpha clusters in the tetrahedron and octahedron respectively. The best overall fit is with \( \alpha = 1.7 \text{ fm} \), \( R_1 = 2.2 \text{ fm} \) and \( R_2 = 3.9 \text{ fm} \). If one changes \( R_1 \) and \( R_2 \) to \( 2.1 \text{ fm} \) and \( 3.6 \text{ fm} \), the first two maxima are better reproduced, but the fit above \( 2.0 \text{ fm}^{-1} \) is destroyed. The agreement between theory and experiment is also improved if one introduces a fourth parameter by allowing the rms radii of the inner and outer alpha clusters to differ. It is interesting to note that the second minimum of the theoretical curve does not go to zero. This fact leads to some interesting results that will be examined more closely in the next section.
1. Mass Shapes and Charge Distributions

As a result of the calculations in the preceding section, the CAP model can now predict the position and rms radius of each internal alpha cluster for all nuclei listed in the first column of Table 2.17. Thus it is possible to calculate classically the "rigid" moments of inertia for these nuclei and compare them to the "effective" moments that are needed to reproduce their energy spectra. Table 2.17 compares the "effective" and "rigid" rotational parameters which vary as the reciprocal of the moments. In order to make the calculations more realistic, the center α-clusters of $^{20}\text{Ne}$ and $^{28}\text{Si}$ were assumed not to contribute to the "rigid" moments of inertia. From Table 2.17, one sees that the "rigid" moments are usually twice as large as the "effective" moments for rotations about the $x$ or $y$ axis, and three to four times as large for rotations about the symmetry axis. This is not unexpected since a similar situation occurs for deformed nuclei in the regions $150 \leq A \leq 190$ and $A \geq 220$ (41, p. 288).

Finally, we calculate the effective radial charge distribution for several different nuclei by averaging the charge distribution of Equation 2.32 over all possible orientations. This is accomplished by taking the inverse Fourier transform of the elastic scattering form factor. From Equations 2.58 and 2.60, we find

$$ F_{00}^\dagger = \frac{e^{-g_2a^2/6}}{\gamma} \sum_{n=1}^{n} \mathcal{F}_n(g, R, z), $$

and a straightforward integration yields

$$ \rho(r) = \frac{2e}{\alpha^2} \sqrt{\frac{3}{2\pi n^2}} \sum_{n=1}^{n} \left( \frac{1}{R_n} \right) \exp \left[ -3(y^2 + R_z^2) \right] \sinh \frac{3R_z r}{\alpha^2}. $$
Table 2.17. Comparison of "rigid" and "effective" rotational parameters for several light nuclei. The spatial parameters needed to calculate the 'rigid" A_j's were found by applying the CAP model to electron scattering data.

<table>
<thead>
<tr>
<th>Assumed α-structure</th>
<th>Levels used in calculating &quot;effective&quot; rotational parameters</th>
<th>Calculated rotational parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>&quot;Effective&quot; (MeV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>A1=A2</td>
</tr>
<tr>
<td>9^9Ne</td>
<td>D_{ωh} dumbbell with neutron</td>
<td>5/2^- 2.43 MeV</td>
</tr>
<tr>
<td>12^12C</td>
<td>D_{3h} equilateral triangle</td>
<td>2^+ 4.43 MeV</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3^- 9.64 MeV</td>
</tr>
<tr>
<td>16^16O</td>
<td>T_d tetrahedron</td>
<td>3^- 6.13 MeV</td>
</tr>
<tr>
<td>20^20Ne</td>
<td>D_{2d} distorted tetrahedron</td>
<td>2^+ 1.63 MeV</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2^- 4.97 MeV</td>
</tr>
<tr>
<td>24^24Mg</td>
<td>D_{2h} bitetrahedron</td>
<td>2^+ 1.37 MeV</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2^+ 4.23 MeV</td>
</tr>
<tr>
<td>28^28Si</td>
<td>Oblate D_{3d} structure</td>
<td>2^+ 1.78 MeV</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3^+ 6.27 MeV</td>
</tr>
</tbody>
</table>
where $\rho(r)$ is the radial charge distribution of the nucleus normalized to the proton charge, $2ne$.

Figure 2.27a, taken from Reference (31), shows the radial charge distributions for alpha-particle configurations of $^{12}\text{C}$ and $^{16}\text{O}$. The $D_{5h}$ curve in Figure 2.27c is computed from parameters given in Reference (35); this distribution also fits the experimental $|F_0^+|^2$ for $^{28}\text{Si}$ (given in Figure 2.22a). The phenomenological fit to $^{40}\text{Ca}$ in Figure 2.27d is taken from Reference (83). All other curves are calculated from parameters given in the present paper. The two charge distributions for $^{28}\text{Si}$ have essentially the same absolute elastic form factor up to 1.8 fm$^{-1}$, but they can be shown to vary considerably above this value. In particular, the third maximum of $|F_0^+|^2$ for the $D_{3d}$ structure is calculated to 100 times as large as that of the $D_{5h}$ case. Future experiments on the elastic scattering form factors of $^{28}\text{Si}$ at higher energies will thus favor one distribution over the other. On the other hand, the absolute form factor curve for $^{40}\text{Ca}$ is known well up to 3.2 fm$^{-1}$, and both distributions of Figure 2.27d give approximately the same $|F_0^+|$ through the fourth maximum. The large difference in the two distributions is thus probably due to the fact that the phenomenological fit assumes the form factor changes sign at the second minimum (as shown in Reference (82)), whereas the form factor for the $\pi$-structure does not (c.f. Figure 2.26c). Although the absolute values of the form factors of the two distributions are nearly the same, the actual form factors are quite different above 2.0 fm$^{-1}$. In fact, by slightly altering the present charge distribution, which is somewhat hollow in the center, one should be able to calculate differential cross-section curves just as good as those obtained for the previous phenomenological distribution. Since the Born approximation can no
Figure 2.27. Radial charge distributions of various light A=4N nuclei predicted by the CAP model. The assumed structure of each nucleus is also given.
longer be used for such an exact calculation, no attempt is made at present to validate this assumption.

J. Comparison with Other Models

From the results of the last two sections, it appears that the CAP model works quite well for even-even nuclei up to the middle of the 2s-1d shell, but has only moderate success for the nuclei above $^{28}$Si. The only logical $\alpha$-structures for the three $A=4N$ nuclei in the 1p shell yield results in quite good agreement with experiment. Also, some of the discrepancies that do occur between experiment and theory can be reasonably well explained by considering the more realistic RAP model.

For even-even nuclei in the 2s-1d shell, several $\alpha$-structures are possible for each nucleus, and the physical structure must be determined from analyzing the available data. All of the observed $K^\pi$ bands of $^{20}$Ne under 9 MeV can be predicted with the $D_{2d}$ distorted tetrahedron, and the levels of $^{24}$Mg are well-described by the $D_{2h}$ bitetrahedron. The results for $^{28}$Si are not as conclusive as for the previous two nuclei, though present data favor an oblate $D_{3d}$ structure over the more familiar $D_{5h}$ pentagonal bipyramid. The structures assumed for $^{24}$Mg and $^{28}$Si both give good agreement with the experimental electron scattering form factors. Several structures do a fair job in predicting the energy levels of $^{32}$S and $^{36}$Ar. However in both of these nuclei, low-lying levels are observed that are not well predicted. The nucleus $^{40}$Ca is found to have an $\alpha$-structure of $O_h$ symmetry. Although the energy spectrum is only qualitatively discussed, the experimental elastic form factor for electron scattering is well described. For nearly all of the $A=4N$ nuclei considered in the 2s-1d shell, the first energy level
observed but not predicted is usually a $3^-$ state. These levels may have some contribution from an octopole vibration which is not part of the CAP model.

In recent years, deformed Hartree-Fock (DHF) (8, 84-87), SU$_3$ (88, 89), intermediate-coupling (90-92), and unified collective models (58, 93, 94) have all been applied to most of the even-even nuclei with atomic mass A$\approx$40. The DHF calculations usually allow the nucleus to have only axial or ellipsoidal (i.e. D$_{2h}$ symmetry) deformations (8, 84). However, even with these restricted deformations, some interesting comparisons with the CAP model can be made. The ground-state DHF structures for $^{20}$Ne and $^{24}$Mg are definitely prolate, but an oblate structure is found to be slightly favored in $^{28}$Si. These results are in good agreement with experiment (c.f. Table 2.10) as well as with our structures. In addition, $^{24}$Mg appears to prefer an ellipsoidal rather than an axially symmetric shape; this qualitatively agrees with our D$_{2h}$ bitetrahedron (Figure 2.16c). Ripka (8, p. 254) has plotted some very informative density distribution curves for his axially symmetric DHF solutions of $^{12}$C, $^{20}$Ne, and $^{28}$Si. The irregularities in the equidensity surface show good evidence for four-body correlations in all three nuclei. For example, $^{12}$C is shown to be oblate and hollow in the center (i.e. toroidal shaped), which is in close agreement with the triangular $\pi$-structure assumed by the CAP model. Such a deformed shape for $^{12}$C also gives a definite increase in binding energy over the best spherical HF solution (95; 96 p. 259). The density plot of $^{20}$Ne seems to differ from the results of the present work as it favors the D$_{3h}$ bipyramid (Figure 2.10c) over the D$_{2d}$ distorted tetrahedron (Figure 2.10a). One possible explanation for this discrepancy is that D$_{2d}$ distortions were not allowed in the DHF calculations. Unfortunately no density plot was drawn for $^{24}$Mg.
The previous section shows how the CAP model gives an especially simple explanation for the opposite parities of the $K=2$ bands in $^{20}\text{Ne}$ and $^{24}\text{Mg}$. As noted before, other collective models, especially the asymmetric rotor (93), can account for the $K^\pi=2^+$ band in $^{24}\text{Mg}$, but the negative-parity bands in $^{20}\text{Ne}$ are usually explained by promoting the $1p$-shell nucleon to the $2s-1d$ shell. In the unified Nilsson model, this promotion results in several different bands (94), and it is difficult to tell which ones are lowest in energy. This difficulty is removed in the $SU_3$ model because one assumes that the lowest states are those of maximum orbital symmetry. Thus the negative-parity states of $^{20}\text{Ne}$ are presumed to be built on the $[\lambda\mu]=[82]$ or $[90]$ irreducible representations of $SU_3$; the former is a five-particle one-hole state, while the latter is obtained on promoting a $2s-1d$ shell nucleon to the next higher shell. Using Elliott's projection scheme (97), one finds that the $[82]$ space yields $K^\pi=2^-$ and $K^\pi=0^-$ (L even) bands, while the $[90]$ space has only a $K^\pi=0^-$ (L odd) band. The first and third bands are observed experimentally (Figure 2.11), but they are also explained by the CAP in a quite different manner. The $SU_3$ model can also explain the $K^\pi=0^+$ and $K^\pi=2^+$ bands of $^{24}\text{Mg}$ as belonging to the $[\lambda\mu]=[84]$ irreducible representation. Harvey (88, p. 96) has plotted the particle probability density distribution for the intrinsic part of this particular state; the contour lines again show correlation and seem to favor the $D_{2h}$ bitetrahedron of Figure 2.16c.

Finally, we shall compare our $\alpha$-structures found for the $A=4N$ nuclei in the $2s-1d$ shell with those configurations that have been considered by various $\alpha$-cluster calculations. The "resonating group method" formulated by Wheeler in 1937 has been extended by numerous authors in recent years (47, 98-100). Unfortunately, the calculations involve an exact variational method.
and become extremely complicated when more than two clusters are considered. The calculations are therefore usually limited to such nuclei as $^6\text{Li}$, $^7\text{Be}$, $^7\text{Li}$, $^8\text{Be}$. However, at least one calculation has been attempted on $^{12}\text{C}$ with quite favorable results (100). The "generator-coordinate" model proposed by Hargenau (13) makes a simplifying approximation which enables the model to consider $\alpha$-structures for all light $A=4N$ nuclei. The alpha clusters are first assumed to be fixed in the laboratory coordinate system, and the HF calculations are then performed among the many-particle basis functions generated by this stationary configuration (59,101). A quite similar procedure is used in the DHF calculations noted earlier.

Brink and co-workers (59) have recently used the "generator coordinate method" to calculate the binding energies of all $A=4N$ nuclei between $^{12}\text{C}$ and $^{28}\text{Si}$. They find the most stable configurations to be the $D_{3h}$ trigonal bipyramid for $^{20}\text{Ne}$, the $D_{4h}$ square bipyramid for $^{24}\text{Mg}$, and a prolate $D_{3h}$ structure for $^{28}\text{Si}$; the first two are shown in Figures 2.10c and 2.16a respectively. None of these structures is in agreement with the results of the present paper; however, it is not known if our structures for $^{28}\text{Ne}$ and $^{24}\text{Mg}$ were actually considered in their calculations. A number of authors have also searched for $\alpha$-correlations by relaxing the restrictions of the DHF calculations (85-87). Instead of axial or ellipsoidal deformations, they allow for deformations of less symmetry which do not inhibit cluster formations. One of these papers (87) imposed trigonal symmetries on $^{12}\text{C}$, $^{16}\text{O}$, and $^{20}\text{Ne}$, and found alpha correlations in all three nuclei when a Volkov force with a sufficiently strong Majorana exchange term ($M=0.75$ was used. So far as we are aware, no DHF calculation has been performed on $^{20}\text{Ne}$ with $D_{2d}$ symmetry.
The overall results of this chapter seem to indicate that the phenomenological CAP model gives a good basic description of the low-lying levels of several light $A=4N$ nuclei, and it also indicates which symmetries are important for each nucleus. These symmetries should in turn dictate how one can best proceed with more realistic calculations.
III. OTHER TYPES OF COLLECTIVE AND UNIFIED MODELS

As noted in the introduction, the purpose of this chapter is to review the basic theory for the other common collective models and determine what similarities may exist between these models and the CAP model of Chapter II. It will indeed be shown in Section D that two well-known collective models, namely the symmetric and asymmetric rotors, are analogous to two special cases of the CAP model. Then in Section E, the theory will be reviewed for extending the collective symmetric rotor to odd-A nuclei. This review then leads directly to the formulating of a phenomenological $\alpha$-particle model for light $A=4N+1$ nuclei in Chapter IV.

A. Fundamental Assumptions about Nuclear Deformations

Unlike the CAP model, all of the collective models considered in this chapter are derivatives of the liquid drop model and therefore portray the nucleus as a continuous, incompressible fluid. The classical Hamiltonian for a liquid drop had already been worked out in 1877 (102), but it was not until 1952 that A. Bohr perceived how such a system could be quantized and adapted to the nuclear case (103).

The theory for the motions of a deformed liquid drop can be found in many standard texts (41, pp. 262-319; 104, pp. 228-291), and only a very brief review of the derivation will be given at present. One begins by expanding the surface of the drop in terms of spherical harmonics as

$$ R(\theta, \phi) = R_0 \left[ 1 + \sum_{\ell m} \alpha_{\ell m} Y_{\ell m}^{*}(\theta, \phi) \right] . \tag{3.1} $$

In the nuclear case, the surface is not well defined, so $R(\theta, \phi)$ is taken to be a surface of constant density. Assuming small oscillations of the core,
one can show after some calculation that
\[ H(a, \hat{a}) = \frac{1}{2} \sum_{x} B_{x} a_{x}^{*} a_{x} + \frac{1}{2} \sum_{x} B_{x} \omega_{x}^{2} a_{x}^{*} a_{x} . \] (3.2)

Only lowest order terms in \( a \) and \( \hat{a} \) have been kept. The above Hamiltonian holds for any surface vibration. However, the coefficients \( B_{x} \) and \( B_{x} \omega_{x}^{2} \) depend on basic assumptions concerning the nature of the liquid, which is normally considered to be an incompressible fluid. The hydrodynamic values for these coefficients are not relevant to the present review and so will not be given.

The Hamiltonian in Equation 3.2 cannot be developed further until one makes some assumptions about the core deformations. Various possibilities exist, and each leads to a different collective model. The more common of these are briefly mentioned in Section B through D.

B. Collective Vibrator Model

If the nucleus vibrates about a spherical equilibrium position, the average value of each deformation parameter \( a_{x} \) is zero, and the Hamiltonian in Equation 3.2 reduces to a sum of simple harmonic oscillators
\[ H(a, \hat{a}) = \sum_{x} H_{x} (a, \hat{a}) , \] (3.3)
where
\[ H_{x} (a, \hat{a}) = \frac{1}{2} B_{x} \left[ |a_{x}|^2 + \omega_{x}^2 |a_{x}|^2 \right] . \] (3.4)

The first excited state of each mode is \((2L+1)\)-fold degenerate, and so has spin \( L \) and parity \((-)^{L}\). Inserting the hydrodynamic values for \( B_{x} \) and \( B_{x} \omega_{x}^{2} \), one finds the vibrational quantum \( \tilde{\omega}_{x}^{2} \) to be a monotonically increasing function of \( x \) with \( \tilde{\omega}_{0}^{2} = \tilde{\omega}_{1}^{2} = \tilde{\omega} \), and \( \tilde{\omega}_{x}^{2} = 2 \tilde{\omega}_{2} \). The first excited state of a
vibrator nuclei should therefore have spin $2^+$ with energy $\hbar \omega_2$. Then at about twice this energy, there should be a $3^-$ state at $\hbar \omega_3$ as well as a $0^+, 2^+, 4^+$ triplet at $2\hbar \omega_2$ arising from two phonons of the quadrupole vibration. Many nuclei exhibit this type of spectrum including $^{32}$S and $^{36}$Ar (c.f. Figures 2.23 and 2.24), but the experimental $\hbar \omega'$s are normally only half of the hydrodynamic estimates.

C. The Collective Rotor-Vibrator Model

Some nuclei are known to have large intrinsic quadrupole moments. For such nuclei, at least one of the core deformation parameters, $a_{20}$, has a large nonzero equilibrium value, and much of the kinetic energy in Equation 3.2 will then come from the collective rotations of the $a_{\ell m}$'s. In describing the motions of permanently deformed nuclei, it becomes advantageous to characterize the deformations in terms of a body-fixed coordinate system. The Euler angles that describe the orientation of these body axes are identical to those in the previous chapter and are defined in Figure 2.1.

The lowest-lying positive parity states should be generated by the nontrivial deformation, $\ell=2$. Thus in the body coordinates, one has

$$R(\phi', \phi') = R_0 \left[ 1 + \sum_m a_{2m}^b Y_{2m}^* (\phi', \phi') \right], \quad (3.5)$$

where the primes indicate that the expansion is carried out in body coordinates. The Hamiltonian, which can be simply expressed in laboratory coordinates as

$$H(a, \dot{a}) = \frac{i}{2} B_2 \left\{ \frac{1}{2} |a_{2m}|^2 + \omega_2 |a_{2m}|^2 \right\}, \quad (3.6)$$

must be transformed to body coordinates, since only there does one have some
idea of how the deformation parameters vary in time. The transformation is elegant but quite involved and will not be presented in this work. We merely note that the resultant Hamiltonian is greatly simplified if one imposes the following three limitations on the body deformation parameters

\[ a_{2,2} = a_{2,2}, \quad a_{2,1} = a_{2,-1} = 0, \quad (3.7) \]

and redefines the remaining two nonzero deformations as

\[ a_{2,0} = \beta \cos \gamma, \quad a_{2,2} = \sqrt{\frac{\gamma}{2}} \beta \sin \gamma, \quad (3.8) \]

The conditions of Equation 3.7 arise naturally from requiring the body axes to coincide with the principle axes of the rotating structure. The surface of the drop then has the form

\[ R(\phi, \phi') = R_0 \left[ 1 + \beta \{ \cos \gamma \left( \phi - \phi' \right) + \sqrt{\frac{\gamma}{2}} \sin \gamma \left[ \gamma_{22} \left( \phi - \phi' \right) + \gamma_{2,2} \left( \phi - \phi' \right) \right] \} \right], \quad (3.9) \]

and the Hamiltonian can be written as

\[ H = \frac{3}{2} \frac{\hbar^2 L^2}{2 I^2} + \frac{1}{2} B_2 \left( \beta^2 + \beta^2 \gamma^2 \right) + \frac{1}{2} B_2 \omega^2 \beta^2, \quad (3.10) \]

which is comparable to the Hamiltonian for the CAP model (Equation 2.2).

The hydrodynamic values for the moments of inertia are

\[ I^2 = \frac{3}{2 \pi} M R_0^2 \beta^2 \sin^2 \left( \phi - \frac{2 \pi}{3} \right), \quad \kappa = 1, 2, 3, \quad (3.11) \]

(Where \( M \) is the mass of the nucleus), and are usually much smaller than the ones needed to fit experimental data.
The rotation-vibration models that have resulted from various approximate solutions of Equation 3.10 have had remarkable success for many even-even nuclei in the mass regions $150 < A < 180$ and $A < 220$. These models can be grouped into two broad classes depending upon whether the equilibrium position of the nucleus is axially symmetric (105) or not (106). Many of these models make at least the following two assumptions.

1. The rotation-vibration interactions are neglected by assuming that the moments of inertia $I_K$ are constants evaluated at the equilibrium positions of $\beta$ and $\gamma$.

2. The strong anharmonic terms in the potential are considered only qualitatively by allowing the rotational parameters, $A_K = \pi^2/2I_K$, to acquire smaller values for higher vibrational modes.

Both of these approximations were made with about equal validity in the CAP model (Section II A).

D. Static Rotor Models

We shall finally consider two limiting cases of the rotor-vibrator model which assume that the deformation parameters $\beta$ and $\gamma$ are constants, so that vibrations do not have to be considered. Two types of rotors exist depending upon whether the asymmetry parameter $\gamma$ is zero or finite. The levels predicted by both of these rotors will be found to correspond to the ground state rotational band of two distinct symmetries of the CAP model.

1. **Asymmetric rotor**

   The asymmetric rotor occurs when the parameter $\gamma$ is not zero. The surface in body coordinates can then be written as
where $\beta$ and $\gamma$ are now constants independent of time. In general, the three moments of inertia will all be different (c.f. Equation 3.11) so that the eigenstates of the rotor Hamiltonian

$$H = \sum A_K \mathbf{L}_K^2$$

will necessarily belong to one of the IR's of $D_{2h}$ as has already been discussed in the previous chapter for $^{24}_{\text{Mg}}$. Experimentally, only $A_{1g}$ levels are observed and one must therefore give some arguments for why $A_{1g}$ levels occur and all others vanish. In the CAP model, this was easily accomplished in a rigorous manner by invoking Bose-Einstein statistics (Section 11B); but this method cannot be used in the present case since no alpha clusters are present. The usual argument given in most standard texts was originally stated by Bohr, who indicated that since the Hamiltonian was spatially invariant under $D_{2h}$, the wavefunctions must also be so (104, p. 239). Such a statement is not true since the invariance of a Hamiltonian under a particular group simply implies that the eigenvectors must belong to one of many IR's of the group. Davidson objects to this argument in a later review article (3) and selects the wavefunctions of the $A_{1g}$ IR as the physical ones simply because they agree with experiment. The spectrum of the asymmetric rotor is therefore identical to that of the ground state rotational spectrum for an $\alpha$-structure having $D_{2h}$ symmetry.

2. **Symmetric rotor**

If the asymmetry parameter $\gamma$ is zero, the rotor reduces to that of a symmetric rotor. The surface of the nucleus can now be written as
and the explicit forms of the three moments of inertia can be calculated from Equation 3.11 to be

\[ I_1 = I_2 = \frac{9}{8} \pi z M A_o^2 \beta \]
\[ I_3 = 0 \]

The rotational Hamiltonian for the symmetric top is

\[ H = A_1 (L_z^2 + L_\varphi^2) + A_2 L_\varphi^2 \]

But the rotational parameter \( A_2 = \frac{h^2}{2I_3} \) is infinite and so the eigenfunctions \( D_{JK}^{1/2}(\pi) \) must have \( K=0 \). The projection of the angular momentum on the body-fixed \( z \) axis, \( L_z \), must therefore be zero, and the Hamiltonian simplifies to

\[ H = A_1 L_z^2 \]

To agree with experiment, one must further reduce the allowed states to those invariant under a rotation of 180° about an axis in the \( xy \) plane.

This is usually accomplished by employing Bohr's argument, which has already been shown to be not entirely valid. The allowed spectrum then includes only a \( K=0^+ \) band with even parity states, and is identical to an \( \chi \)-structure having \( D_{ooh} \) symmetry, as was illustrated in the previous chapter for \(^8\text{Be}\).

E. Unified Symmetric Rotor

The collective vibrator model and the symmetric and asymmetric rotors have all been extended in the unified sense so that they might also describe the levels of odd-\( A \) nuclei. All three models have met with a great deal of success in various mass regions of nuclei, but for the present we shall
review only the derivation of the unified symmetric rotor since this is all that is needed for developing the unified $x$-particle model of Chapter IV. The present derivation will deviate somewhat from Nilsson's original paper (107), as well as from standard texts, since we will be concerned only with those parts which have direct application in the next chapter. However, unlike the preceding sections, those areas which are relevant to Chapter IV will be developed in great detail.

1. Hamiltonian and basis functions for extra-core particle

We begin by writing the total Hamiltonian as

$$H = H_A + H_p$$  \hspace{1cm} (3.18)

The core Hamiltonian is the same as that of the collective symmetric rotor given in Equation 3.17, which is

$$H_A = A \lambda^2$$  \hspace{1cm} (3.19)

The periods of particle motion are somewhat greater than those of collective rotations, so it becomes convenient to solve the single-particle Hamiltonian in body coordinates. The particle Hamiltonian can be written as

$$H_p = \frac{P^2}{2m} + V(r', \phi', \phi')$$  \hspace{1cm} (3.20)

In order to find a suitable potential, we note from Equation 3.14 that

$$r'(\phi', \phi') = r\left[1 + \beta \xi_0 \left(\phi', \phi'\right)\right]$$  \hspace{1cm} (3.21)

One can also think of $r(\phi', \phi')$ as a surface of constant potential as well as a surface of constant density. The potential along this surface can be
written as

\[ V_0 = \frac{1}{2} m \omega_o^2 \gamma^2 = \frac{1}{2} m \omega^2 (\phi', \phi') \gamma^2 (\phi', \phi') . \]  

(3.22)

From Equation 3.21, we have to first order in \( \beta \)

\[ \gamma^2 (\phi', \phi') = \gamma^2 \left[ 1 + 2 \beta \gamma_2^*(\phi', \phi') \right] . \]  

(3.23)

Therefore, in order for Equation 3.22 to hold to first order in \( \beta \), one must have

\[ \omega^2 (\phi', \phi') = \omega_o^2 \left[ 1 - 2 \beta \gamma_2^*(\phi', \phi') \right] , \]  

(3.24)

and the deformed potential is then

\[ V(\theta', \phi') = \frac{1}{2} m \omega^2 (\theta', \phi') \gamma^2 \]  

\[ = \frac{1}{2} m \omega_o^2 \gamma^2 \left[ 1 - 2 \beta \gamma_2^*(\phi', \phi') \right] . \]  

(3.25)

(3.26)

Besides the above potential, the above particle Hamiltonian has a spin-orbit term as well as an \( L^2 \) term which interpolates the potential between a harmonic oscillator and a square well. The particle Hamiltonian of Equation 3.20 then becomes

\[ H_p = -\frac{\hbar^2 \nabla^2}{2m} + \frac{1}{2} m \omega_o^2 \gamma^2 \left[ 1 - 2 \beta \gamma_2^*(\phi', \phi') \right] + c \xi \cdot \xi + d \xi^2 . \]  

(3.27)

By introducing the dimensionless coordinates

\[ \rho^2 = \frac{m \omega_b}{\hbar} \gamma^2 , \]  

(3.28)

\[ \nabla \rho^2 = \frac{\hbar}{m \omega_b} \nabla^2 . \]  

(3.29)

Equation 3.27 simplifies to
The parameters $\chi$ and $\mu$ are similar to the ones Nilsson defined in his original paper. From Equations 3.27 and 3.30, one can show

$$\chi = -\frac{c}{2\pi \omega_0}$$

(3.31)

$$\mu = -\frac{D}{\chi \pi \omega_0} \quad .$$

(3.32)

The parameter $\hbar \omega_0$ is normally taken to be a fitting parameter, but should be approximately (49, p. 469)

$$\hbar \omega_0 = \frac{1}{2} \frac{A}{A^{1/2}} \ \text{MeV} \quad .$$

(3.33)

A suitable set of basis functions for diagonalizing the particle Hamiltonian is the spherical harmonic oscillator wavefunctions $|N\ell \ell \ell m\ell \rangle$ (the quantum numbers are defined in Appendix E). A straightforward calculation shows that the matrix elements are

$$< N\ell' \ell' \ell' \ell' m' | H_p | N\ell \ell \ell \ell m \rangle = \frac{\hbar \omega_0}{\pi} \sum_{\ell_3} \sum_{m_3} \sum_{m_3} \sum_{m_3} \hbar \omega_0 [N + \frac{3}{2} - 2\chi \frac{\ell (\ell + 1) - s (s + 1) - \ell \ell (\ell + 1) - \ell (\ell + 1)}{2}]

+ (-)^{\ell_3 - \ell_3'} \frac{\beta_2 \hbar \omega_0}{\pi} \sum_{\ell_3} \sum_{m_3} \sum_{m_3} \hbar \omega_0 [N + \frac{3}{2} - 2\chi \frac{\ell (\ell + 1) - s (s + 1) - \ell \ell (\ell + 1) - \ell (\ell + 1)}{2}]

\times \langle \ell' \ell' \ell' \ell' m' | \rho^2 | N\ell \ell \ell \ell m \rangle \langle \ell' \ell' \ell' \ell' m' | \ell' \ell' \ell' \ell' m' \rangle \quad .$$

(3.34)

The eigenvalue problem can be greatly simplified by diagonalizing $H_p$ only among basis states of a particular IR for $D_{\infty h}$. These IR's can be uniquely identified by the absolute value of $m$ and parity, $\pi$. Since $m$ is always half-integral, all the IR's will be doubly degenerate.

The resultant pair of wavefunctions found after diagonalization for an IR of quantum numbers $|m| \rangle$ and $\pi$ can be written as a spinor in the form

$$|\lambda, \pi, m\rangle \quad \text{where} \quad \lambda \text{ is an ordinal number that distinguishes levels of the}$$

$$|\lambda, \pi, -m\rangle \quad .$$
same IR. One might expect that these spinors can be expanded in the following pairs of spherical wavefunctions: \((N_{\ell s} j m \rangle, N_{\ell s} j, m')\). This, however, can be shown not to be the case by considering \(C_2^x\) rotations on these spinors. From Equation B11, one finds

\[ C_2^x \langle \ell j m \rangle = e^{-i\pi/2} \langle \ell j, -m \rangle, \tag{3.35} \]

and so the matrix representation for \(C_2^x\) using the above set of spherical basis functions is \(\begin{pmatrix} 0 & e^{-i\pi j} \\ e^{-i\pi j} & 0 \end{pmatrix}\), a matrix that depends explicitly on \(j\). This is not appropriate for the present situation because all matrix representations of rotations of the diagonalized wavefunctions \((|\lambda \pi m \rangle, |\lambda \pi, -m \rangle\) must be independent of \(j\). One possible solution is to choose the spherical basis functions in the form \((\pm j + 1/2 |N_{\ell s} j m \rangle)\). This extra phase now causes the \(C_2^x\) representation to be

\[ \begin{pmatrix} e^{i\pi j/2} & \circ \\ \circ & e^{-i\pi j/2} \end{pmatrix} = \begin{pmatrix} 0 & e^{i\pi j/2} \\ e^{i\pi j/2} & 0 \end{pmatrix}, \tag{3.36} \]

a matrix independent of \(j\). For later use, we note from Equation B10 and the above discussion that

\[ C_2^z(\phi) |\lambda \pi m \rangle = e^{-i\lambda m \phi} |\lambda \pi m \rangle \tag{3.37} \]

and

\[ C_2^x |\lambda \pi m \rangle = e^{i\pi/2} |\lambda \pi, -m \rangle, \tag{3.38} \]

where \(C_2^z(\phi)\) is an arbitrary rotation of angle \(\phi\) about body-fixed \(z\) axis. In addition, the resultant wavefunctions can now be expanded in the spherical basis as

\[ |\lambda \pi m \rangle = \sum_{\mu} C_{\lambda \mu} |\lambda \mu, m \rangle \sum_{\mu'} C_{\lambda \mu'} |\lambda \mu', m \rangle, \tag{3.39} \]
The phase difference, \((-)^{J+1/2}\), in the two expansion coefficients will be of extreme importance when one couples the particle and core wavefunctions.

The results of a typical diagonalization of \(H_p\) are shown in Figure 3.1 where the single-particle energy levels up through the 2s-1d shell are plotted as a function of the deformation parameter, \(\beta_2\). Not all of the single-particle levels in this figure are allowed as possible states for the extra nucleon. The lower levels are assumed filled by the core nucleons, and the Pauli exclusion principle prevents the last particle from entering the core states. The nucleus \(^{13}\text{C}\) is shown as an example; each level is doubly degenerate and can therefore hold two protons and two neutrons, so the lowest three single particle levels are filled with core nucleons. The last proton can then only occupy the states higher than these core levels.

2. Coupled basis functions

One must now obtain a suitable coupled basis for diagonalizing the total Hamiltonian of Equation 3.18. Figure 3.2 shows the possible angular momenta that are involved in the coupling of the core and particle. The following sum rules hold on the quantum numbers,

\[
I = J' + L', \quad M = m' + M_L
\]  

(3.41)

(3.42)

and

\[
M = m + M_L
\]  

(3.43)

As shown in the figure, the parameters \(K, m'\) and \(K_L\) are defined in the
Figure 3.1. The single particle energy levels of H (given in Equation 3.30) are plotted as a function of the deformation parameter $\beta_2$. The $\xi$ and $\eta$ coefficients, $\lambda_0$ and $\chi_0$, have values of 0.15 and 0.0 respectively. The Pauli-exclusion principle is also demonstrated by showing the states that are filled for $^{13}$C. The last neutron cannot occupy the lower three "core" levels.
Figure 3.2. The angular momentum coupling relations for a deformed core plus particle Hamiltonian.
body-fixed coordinates while $M$, $m$ and $M_L$ refer to the laboratory system.
The only quantum numbers that are conserved in the final wavefunctions are
total spin ($I$), its projection on the space-fixed $z$ axis ($M$), and parity ($\pi$).
One such wavefunction satisfying these conditions can be formed in the labo­
rary where the usual angular momentum coupling holds

$$
<y_1, \alpha | N L S_j; \ell, \ell_m; \ell M > \equiv \sum \sum \text{e}^{i \ell L; m M L M} \langle N | N S_j m \rangle \frac{D^{L}_{M M L} (\alpha)}{N_L} .
$$

The first term on the right-hand side is the usual Clebsch-Gordan coeffi­
cient. In the second term, $\Sigma$ represents all coordinates of the particle
wavefunction in space-fixed coordinate system, and $| N S_j m \rangle$ denotes the
single-particle spherical harmonic oscillator with quantum numbers $N S_j m$ (as
defined in Appendix E). The last terms represent the core wavefunction and
$N_L$ is the normalizing factor $N_L = \frac{2L+1}{8\pi^2}$.

These wavefunctions cannot be used as basis functions, however, because
the particle wavefunction is described in body coordinates (Equation 3.20).
This problem can be remedied by transforming the particle wavefunction to
body coordinates (via Equation A2) and then using the Clebsh-Gordan series
for the rotation matrices and symmetry and unitarity properties of the
Clebsch-Gordan coefficients:

$$
<y_1, \alpha | N L S_j; \ell, \ell_m; \ell M > \equiv \sum \sum \text{e}^{i \ell L; m M L M} \langle N | N S_j m \rangle \frac{D^{L}_{M M L} (\alpha)}{N_L} .
$$

$$
= N_L \sum \sum \text{e}^{i \ell L; m M L M} \langle N | N S_j m \rangle D^{L}_{M M L} (\alpha) \frac{D^{L}_{M M L} (\alpha)}{N_L} .
$$

$$
= N_L \sum \sum \text{e}^{i \ell L; m M L M} \langle N | N S_j m \rangle \frac{D^{L}_{M M L} (\alpha)}{N_L} .
$$

$$
= N_L \sum \sum \text{e}^{i \ell L; m M L M} \langle N | N S_j m \rangle \frac{D^{L}_{M M L} (\alpha)}{N_L} .
$$

$$
= N_L \sum \sum \text{e}^{i \ell L; m M L M} \langle N | N S_j m \rangle \frac{D^{L}_{M M L} (\alpha)}{N_L} .
$$
The product wavefunctions on the right hand side of the last equation are close to being the appropriate ones needed to use for the coupled basis functions. The variables I and M are good quantum numbers, and the particle wavefunction is represented in body coordinates. In addition, they are a complete set, since one can invert the last equation to obtain

\[
\langle \gamma', \alpha | N \epsilon S \delta^j m_j^l ; KIM \rangle \equiv \langle \gamma' | N \epsilon S \delta^j m_j^l \rangle N_\chi D_{MK}^{\chi} (\alpha) 
\]

We now assume that the coupled basis functions cannot allow the particle to contain single particle contributions of the core; so instead of the wavefunctions in Equation 3.46, we use

\[
\langle \gamma', \alpha | \lambda \eta m \delta^j m_j^l ; KIM \rangle \equiv \langle \gamma' | \lambda \eta m \delta^j m_j^l \rangle N_\chi D_{MK}^{\chi} (\alpha) 
\]

For reasons that are identical to those used in the collective symmetric rotor (Section IIIID), we again require the coupled basis functions to belong to the symmetric IR of \(D_{\alpha h}^{\gamma} \). The wavefunctions \(D_{MK}^{\chi} \) and \(| \lambda, \eta, \pm m \rangle \) each generate individual IR's of \(D_{\alpha h}^{\gamma} \) labeled by \([K, \eta] \) and \([m, \eta] \) respectively. From group theory, we know that the tensor product of two IR's within the same group will contain the symmetric IR of the group once if and only if the IR's are the same. In the present case, this stipulates that \(K=m \).

In order to find these symmetric wavefunctions, we use Equations B6, B7, 3.37, and 3.38 to show that the coupled wavefunctions of Equation 3.47 transform as
\[ C^c(\phi) |2^\pi m; KIM\rangle = e^{-i\phi(K-m)} |2^\pi m; KIM\rangle \]  
\[ C^x |2^\pi m; KIM\rangle = e^{-i\pi(x+\frac{1}{2})} |2^\pi m; KIM\rangle . \]

From Equation 3.47, one sees that the product wavefunction is invariant under \( C^c(\phi) \) only if \( K=m \) (as has already been noted). In order for the basis function to be invariant under \( C^x \), one must use the combination
\[
|2^\pi lm; KIM\rangle = \sqrt{\frac{3}{2}} \left[ |2^\pi m; KIM\rangle + (-)^{x+\frac{1}{2}} |2^\pi -m; -KIM\rangle \right]^2 ,
\]  
which can be rewritten using Equation 3.39
\[
|2^\pi lm; KIM\rangle = \sqrt{\frac{3}{2}} \sum_{\beta_2, \nu, \mu} C_{\nu s \delta} (\beta_2, \nu, \mu) \nonumber
\]
\[
\times \left[ |Nl s \delta m; KIM\rangle + (-)^{x+\frac{1}{2}} |Nl s \delta -m; -KIM\rangle \right] . \]

3. **Calculating the final energy levels**

The final energy levels are now found by diagonalizing the total Hamiltonian of Equation 3.18 in the coupled basis (Equation 3.50 or 3.51). Using Equations 3.19 and 3.41, one finds the core Hamiltonian to be
\[ H_R = A_1 \left( \frac{1}{2} \sigma_x^2 + \frac{1}{2} \sigma_y^2 \right)^2 , \]  
and the total Hamiltonian can then be expanded as
\[ H = A_1 \left( \sigma_x^2 + \sigma_y^2 \right) - A_1 (I_x \dot{\sigma}_x + I_y \dot{\sigma}_y + I_z \dot{\sigma}_z) + H_P . \]

In his original paper, Nilsson (107) rewrote this expression as
\[ H = H'_R + H'_P + H_{RPR} . \]
He then approximated the Hamiltonian by neglecting $H_{RPC}$ and $A_1 \hat{j}^2$. This left him with a Hamiltonian that was diagonal in the coupled basis of Equation 3.50, and the energy levels were given as

$$E_{\pm m} \propto A_1 \left[ I (I+1) - 2 K^2 \right] + E_{p}^{\pm m},$$

(3.56)

where $E_{p}^{\pm m}$ is one of the particle states of $H_p$. Since $l > K$, this last equation states that a $K$ band of rotational levels with $l = K, K+1, \cdots$ lies on each of the particle energy levels. Kerman improved the theoretical spectrum somewhat by noting that $H_{RPC}$ had diagonal terms when $|K| = 1/2$. His formula for the energy spectrum was then (108)

$$E_{\pm m} \propto A_1 \left[ I (I+1) - 2 K^2 \right] + E_{p}^{\pm m} + \delta_{K, 1/2} \alpha (-)^{I+1/2} (I+1/2),$$

(3.57)

where $\alpha$ is the decoupling parameter which can be shown to be

$$\alpha = \sum_{(\mu \nu \sigma \delta)} (-)^{I+1/2} (I+1/2) \left| C_{\alpha, \mu, \nu, \sigma, \delta} \right|^2.$$

(3.58)

Such a simple expression as Equation 3.57 actually meets with considerable success in many nuclei. However, for light nuclei, it is fairly easy to perform an exact calculation by diagonalizing the Hamiltonian of Equation 3.52 among the basis states of Equation 3.50.

The solid lines in Figure 3.3 show the final energy levels that are obtained as a function of the rotational parameter, $A_1$, assuming that the
Figure 3.3. The solid lines represent the final energy levels of a unified symmetric rotor as a function of the rotational parameter $A_1$. The spins and parities of these levels are given to the top and right of the figure. The particle parameters are the same as those in Figure 3.1, so the energy levels at $A_1=0.0$ are identical to those of Figure 3.1 when $\beta_2=-0.4$. 
particle parameters are the same as those in Figure 3.2 (i.e. $\beta_2 = -0.4$, $2\gamma = 0.15$, $\mu = 0$). If the nondiagonal terms of $H_{RPC}$ and $A_1j^2$ are negligible, the curves will appear as straight lines; this appears to be the case for many of the levels. The dashed lines show the additional levels that are allowed if the core symmetry is reduced from $D_{\infty h}$ to $D_{3h}$ as will be considered in the next chapter.
IV. THE UNIFIED α-PARTICLE MODEL

A. Particle Hamiltonian

The Hamiltonian that we will use for the unified α-particle (UAP) model will again be a sum of core and particle terms,

\[ H = H_C + H_P \]  \hspace{1cm} (4.1)\]

The core Hamiltonian is the same as that used in the CAP model (Equation 2.3) which is

\[ H_C = \sum_{\kappa} A_{\kappa} L_{\kappa}^z \]  \hspace{1cm} (4.2)\]

The particle Hamiltonian will in general no longer have axial symmetry. However, it may be expressed as

\[ H_P = \frac{p^2}{2m} + C \xi \cdot \xi + D \zeta^2 + V(\gamma', \phi', \phi') \]  \hspace{1cm} (4.3)\]

where in analogy to Equation 3.26 we write

\[ V(\gamma', \phi', \phi') = \frac{1}{2} m \omega^2 \gamma'^2 \left[ 1 - \frac{\xi}{x_m} a_{-\kappa}^b y_{\kappa m}^{*} (\theta', \phi') \right] \]  \hspace{1cm} (4.4)\]

Introducing the dimensionless coordinates of Equations 3.28 and 3.29, we find that the last two equations may be written as

\[ H_P = \hbar \omega_0 \left[ -\frac{\gamma^2}{2} - \frac{p^2}{2m} - \frac{x^2}{x_m} a_{-\kappa}^b y_{\kappa m}^{*} (\theta', \phi') - 2 \mu \xi \cdot \xi - \mu \zeta^2 \right] \]  \hspace{1cm} (4.5)\]

where the parameters \( \chi, \mu, \) and \( \hbar \omega_0 \) are defined in Equations 3.31, 3.32, and 3.33. Since the particle Hamiltonian is invariant under all operations of a particular point group, only certain combinations of spherical harmonics are allowed in Equation 4.5. These combinations are listed in Table 4.1 for the
Table 4.1. Lowest order expansion terms of the particle potential for various point group symmetries.

<table>
<thead>
<tr>
<th>Core nucleus</th>
<th>Assumed symmetry</th>
<th>Lowest order nonzero terms in $\sum_{\ell m} a_{\ell m} Y_{\ell m}^* $</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^8$Be</td>
<td>$D_{\infty h}$</td>
<td>$\beta_2 Y_{20}^* + \beta_4 Y_{40}^* $</td>
</tr>
<tr>
<td>$^{12}$C</td>
<td>$D_{3h}$</td>
<td>$\beta_2 Y_{20}^* + \sqrt{1/2} \beta_3 [Y_{32}^* - Y_{3-2}^* ] + \beta_4 Y_{40}^* $</td>
</tr>
<tr>
<td>$^{16}$O</td>
<td>$T_d$</td>
<td>$\sqrt{1/2} \beta_3 [Y_{32}^* - Y_{3-2}^* ] + \beta_4 Y_{40}^* \left{ \sqrt{7/12} Y_{40}^* + \sqrt{5/24} [Y_{44}^* + Y_{4-4}^* ] \right} $</td>
</tr>
<tr>
<td>$^{20}$Ne</td>
<td>$D_{2d}$</td>
<td>$\beta_2 Y_{20}^* + \sqrt{1/2} \beta_3 [Y_{32}^* - Y_{3-2}^* ] + \beta_4 Y_{40}^* + \sqrt{1/2} \beta_4 [Y_{44}^* + Y_{4-4}^* ] $</td>
</tr>
<tr>
<td>$^{24}$Mg</td>
<td>$D_{2h}$</td>
<td>$\beta_2 Y_{20}^* + \sqrt{1/2} \beta_2 ' [Y_{22}^* + Y_{2-2}^* ] + \beta_4 Y_{40}^* + \sqrt{1/2} \beta_4 ' [Y_{42}^* + Y_{4-2}^* ] + \sqrt{1/2} \beta_4 '' [Y_{44}^* + Y_{4-4}^* ] $</td>
</tr>
<tr>
<td>$^{28}$Si</td>
<td>$D_{3d}$</td>
<td>$\beta_2 Y_{20}^* + \beta_4 Y_{40}^* + \sqrt{1/2} \beta_4 [Y_{43}^* - Y_{4-3}^* ] $</td>
</tr>
</tbody>
</table>
various symmetries which were found in Chapter II to yield the best results for A=4N nuclei between $^8\text{Be}$ and $^{28}\text{Si}$. The potential terms given in the last column can be found by standard projection techniques (30, p. 113). The exact form of the potential will depend upon how we choose the body-fixed coordinate system relative to the $\alpha$-structure of the core, so without loss of generality we again choose one of the 2-fold axes in the xy plane to be in the positive x direction.

B. Basis Functions

In accordance with the results of the unified symmetric rotor, we note that the basis functions of the UAP model will involve only half-integral spins and must therefore belong to double-valued IR's of the point group describing the symmetry of the core. Two examples of character tables for such extended point groups are given in Table 4.2 and 4.3. The diagonalized functions of the particle Hamiltonian will now be of the form

$$\left| R_i, l^* \right> = \sum_{(N\ell s j m)} C_{(N\ell s j m)} \left| N \ell s j m \right>,$$

where $i$ denotes the $i^{th}$ double-valued IR of the point-group of interest, and $j$ represents the $j^{th}$ basis function of the degenerate IR. The sum, $(N\ell s j m)$, need only be performed over the spherical basis states $\left| N \ell s j m \right>$ which belong to the IR, $I_i$, and the necessary quantum numbers for each IR of two different point groups are given in Tables 4.4 and 4.5. The results of these tables can be found by the standard reduction procedures given in Section III C. A far simpler method, however, is simply to note which matrix elements of the form $\langle N' \ell' s' j' m' | H_p | N \ell s j m \rangle$ will have a nonzero value. When this occurs,
Table 4.2. Character table for the $D_{3h}$ double-point group.

<table>
<thead>
<tr>
<th>$D_{3h}$</th>
<th>$E$</th>
<th>$R$</th>
<th>$2C_3$</th>
<th>$2RC_3$</th>
<th>$3C_2$</th>
<th>$3C_2'$</th>
<th>$6S_4$</th>
<th>$68S_4$</th>
<th>$6\sigma_d$</th>
<th>$3\sigma_v$</th>
<th>$3\sigma'_v$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$A_1'$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td></td>
</tr>
<tr>
<td>$A_2$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td></td>
</tr>
<tr>
<td>$A_2'$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td></td>
</tr>
<tr>
<td>$E$</td>
<td>2</td>
<td>2</td>
<td>-1</td>
<td>-1</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>$E'$</td>
<td>2</td>
<td>2</td>
<td>-1</td>
<td>-1</td>
<td>0</td>
<td>-2</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>$E''$</td>
<td>2</td>
<td>2</td>
<td>-1</td>
<td>-1</td>
<td>0</td>
<td>-2</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>$E'''$</td>
<td>2</td>
<td>2</td>
<td>-1</td>
<td>-1</td>
<td>0</td>
<td>-2</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>$E''''$</td>
<td>2</td>
<td>2</td>
<td>-1</td>
<td>-1</td>
<td>0</td>
<td>-2</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
</tbody>
</table>

Table 4.3. Character table for the $T_d$ double-point group.

<table>
<thead>
<tr>
<th>$I_d$</th>
<th>$E$</th>
<th>$R$</th>
<th>$6C_3$</th>
<th>$6RC_3$</th>
<th>$3C_2$</th>
<th>$3C_2'$</th>
<th>$6S_4$</th>
<th>$68S_4$</th>
<th>$6\sigma_d$</th>
<th>$6\sigma'_d$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$A_2$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>$E$</td>
<td>2</td>
<td>2</td>
<td>-1</td>
<td>-1</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$T_1$</td>
<td>3</td>
<td>3</td>
<td>0</td>
<td>0</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$T_2$</td>
<td>3</td>
<td>3</td>
<td>0</td>
<td>0</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>$T_1'$</td>
<td>2</td>
<td>-2</td>
<td>1</td>
<td>-1</td>
<td>0</td>
<td>$\sqrt{2}$</td>
<td>-$\sqrt{2}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$T_2'$</td>
<td>2</td>
<td>-2</td>
<td>1</td>
<td>-1</td>
<td>0</td>
<td>$\sqrt{2}$</td>
<td>$\sqrt{2}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$T_3$</td>
<td>4</td>
<td>-4</td>
<td>-1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
Table 4.4. Classification of the body-fixed particle wavefunctions, $\langle \mathbf{r} | j_m \rangle$ for the double-valued IR's of several different point groups. The only quantum numbers given are $j_m$ and $\pi$, with the understanding that all $j_{\pi}|j_m\rangle$ are allowed for each $|j_m\rangle$.

<table>
<thead>
<tr>
<th>IR</th>
<th>$D_{2h}$</th>
<th>$D_{2d}$</th>
<th>$D_{3h}$</th>
<th>$D_{3d}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$j^-$</td>
<td>$\frac{1^+}{2}$, $\frac{3^+}{2}$, $\frac{5^+}{2}$, $\frac{7^+}{2}$, $\frac{9^+}{2}$, $\ldots$</td>
<td>$\frac{1^+}{2}$, $\frac{3^+}{2}$, $\frac{5^+}{2}$, $\frac{7^+}{2}$, $\frac{9^+}{2}$, $\ldots$</td>
<td>$\frac{1^+}{2}$, $\frac{5^+}{2}$, $\frac{7^+}{2}$, $\frac{11^+}{2}$, $\frac{13^+}{2}$, $\ldots$</td>
<td>$\frac{1^+}{2}$, $\frac{5^+}{2}$, $\frac{7^+}{2}$, $\frac{11^+}{2}$, $\frac{13^+}{2}$, $\ldots$</td>
</tr>
<tr>
<td>$j^-$</td>
<td>$\frac{1^-}{2}$, $\frac{3^-}{2}$, $\frac{5^-}{2}$, $\frac{7^-}{2}$, $\frac{9^-}{2}$, $\ldots$</td>
<td>$\frac{1^-}{2}$, $\frac{3^-}{2}$, $\frac{5^-}{2}$, $\frac{7^-}{2}$, $\frac{9^-}{2}$, $\ldots$</td>
<td>$\frac{1^-}{2}$, $\frac{5^-}{2}$, $\frac{7^-}{2}$, $\frac{11^-}{2}$, $\frac{13^-}{2}$, $\ldots$</td>
<td>$\frac{1^-}{2}$, $\frac{5^-}{2}$, $\frac{7^-}{2}$, $\frac{11^-}{2}$, $\frac{13^-}{2}$, $\ldots$</td>
</tr>
<tr>
<td>$j^-$</td>
<td>$\frac{1}{2}$, $\frac{3}{2}$, $\frac{5}{2}$, $\frac{7}{2}$, $\frac{9}{2}$, $\ldots$</td>
<td>$\frac{1}{2}$, $\frac{3}{2}$, $\frac{5}{2}$, $\frac{7}{2}$, $\frac{9}{2}$, $\ldots$</td>
<td>$\frac{1}{2}$, $\frac{3}{2}$, $\frac{5}{2}$, $\frac{7}{2}$, $\frac{9}{2}$, $\ldots$</td>
<td>$\frac{1}{2}$, $\frac{3}{2}$, $\frac{5}{2}$, $\frac{7}{2}$, $\frac{9}{2}$, $\ldots$</td>
</tr>
<tr>
<td>$j^-$</td>
<td>$\frac{1}{2}$, $\frac{3}{2}$, $\frac{5}{2}$, $\frac{7}{2}$, $\frac{9}{2}$, $\ldots$</td>
<td>$\frac{1}{2}$, $\frac{3}{2}$, $\frac{5}{2}$, $\frac{7}{2}$, $\frac{9}{2}$, $\ldots$</td>
<td>$\frac{1}{2}$, $\frac{3}{2}$, $\frac{5}{2}$, $\frac{7}{2}$, $\frac{9}{2}$, $\ldots$</td>
<td>$\frac{1}{2}$, $\frac{3}{2}$, $\frac{5}{2}$, $\frac{7}{2}$, $\frac{9}{2}$, $\ldots$</td>
</tr>
</tbody>
</table>

Table 4.5. Reduction of the basis functions of $\frac{1}{2}$ integral spins of $SU_2$ into the double-valued (denoted by $J^\pi$) into double-valued IR's of $T_d$.

<table>
<thead>
<tr>
<th>IR</th>
<th>$\frac{1^+}{2}$</th>
<th>$\frac{3^+}{2}$</th>
<th>$\frac{5^+}{2}$</th>
<th>$\frac{7^+}{2}$</th>
<th>$\frac{9^+}{2}$</th>
<th>$\frac{11^+}{2}$</th>
<th>$\frac{1^-}{2}$</th>
<th>$\frac{3^-}{2}$</th>
<th>$\frac{5^-}{2}$</th>
<th>$\frac{7^-}{2}$</th>
<th>$\frac{9^-}{2}$</th>
<th>$\frac{11^-}{2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$r^1$</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>$r^2$</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$r^3$</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>2</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>2</td>
</tr>
</tbody>
</table>
it implies that both wavefunctions involved have components which belong to
the same row of the same IR.

In analogy to Equation 3.51, we require the coupled basis functions
that are used for diagonalizing the total Hamiltonian to be special combina­
tions of the product wavefunctions $N_{\lambda}D_{iMK}^{I} (\alpha) |I, j\rangle$. The combinations must
be chosen in such a way that the final wavefunctions are invariant under all
body rotations and reflections which permute identical alpha particles in
the core. From group theory, we know that this requirement limits the al­
lowed rotation matrices, $D_{iMK}^{I} (\alpha)$ to those which belong to the same IR as the
corresponding particle wavefunctions $|I, j\rangle$. Tables 4.4 and 4.5 can still
be used for finding the appropriate rotation matrices if one mentally re­
places the quantum numbers $j$ and $m$ by $I$ and $K$ respectively. The appropriate
set of symmetrized coupled wavefunctions will then be of the general form

$$|IM\pi; I_2\rangle = \frac{N_g}{\sqrt{2}} \leq H_K \left[ \sum_{\ell} G_{a_0} D_{iK}^{I} (\alpha) \right] |I_2, \pi\rangle,$$  \hspace{1cm} (4.7)

where $n_g$ is the dimension of the IR labeled by $I_2$, $G_{a_0}$ are numbers which give
the square braced term the correct symmetry, and $H_K$ are the appropriate
Clebsch-Gordan coefficients. Fortunately, for symmetric tops, the IR's are
all doubly degenerate and it will be shown later that the coupled basis
function for such structures can be simplified to

$$|IM\pi; I_2\rangle = \frac{N_g}{\sqrt{2}} \left[ D_{iK}^{I} (\alpha) |I_2, I\rangle \pm D_{iK}^{I} (\alpha) |I_2, 2\rangle \right]$$ \hspace{1cm} (4.8)

C. Electromagnetic Matrix Elements

1. Extracting reduced matrix elements from experiment

As was stated in Section 11C, the partial mean width of an energy level
for a particular radiation $(\lambda, \phi)$ between states of spin $I$ and $I'$ is
\[
\int \frac{dJ, M}{dJ, M} = \frac{8\pi^{(2\lambda+1)}}{\lambda !(2\lambda+1)!} \left( \frac{E}{\hbar c} \right)^{2\lambda+1} B(\lambda, M; J \rightarrow J') ,
\]

where \( \lambda \) is either E or M depending upon whether the radiation is electric or magnetic, and \( k \) is the rank of the multipolarity. In the present notation, the reduced transition probability will be

\[
B(\lambda, M; J \rightarrow J') = \frac{2\lambda + 1}{4\pi} \left( \frac{2\lambda + 1}{4\pi} \right)^\lambda \sum |<J' M'| \lambda (\lambda, M) | J M >|^2
\]

\[
= \frac{1}{2\pi} |<J' M'| \lambda (\lambda, M) | J M >|^2
\]

and the reduced matrix element is again defined as

\[
<J' M'| \frac{2\lambda + 1}{4\pi} \lambda (\lambda, M) | J M > \equiv <J' M'| \lambda (\lambda, M) | J M >
\]

The calculated transition matrix elements will be much more complicated than for the previously considered \( A=4N \) nuclei, since a significant part of the transition is now produced from the extra-core particle.

Two other measurable quantities which can yield reduced matrix elements are the static magnetic dipole and electric quadrupole moments of the ground state energy level. The necessary relations are

\[
\mathcal{M}_J = \sqrt{\frac{\mu \gamma^2}{3}} \left( \begin{array}{cc} J & J \end{array} \right) <J M \parallel \gamma (I) \parallel J M>
\]

\[
Q_J = \sqrt{\frac{16\pi^2}{5}} \left( \begin{array}{cc} J & J \end{array} \right) <J M \parallel E(2) \parallel J M>
\]

2. The electromagnetic operators

From Equations 4.6 and 4.7, we see that the final wavefunctions will be a sum of terms of the form

\[
<\alpha, J, M; \lambda, M; \lambda', M' > \equiv \mathcal{N}_\lambda <\alpha, M \parallel J \parallel \lambda, M' > D^{\lambda'}_{\lambda, M}(\alpha)
\]
and so the matrix elements that need to be evaluated are of the form

\[ \langle N' \ell' s' \ell' s' | R (R, \mu) | N \ell s \ell s; R \mu \rangle \]  \quad (4.15)

Since the multipole operators are tensors, we find from Equation C20 that they can be expressed as

\[ E (\mathcal{R}, \mu, \nu) = E_z (\mathcal{R}, \mu, \nu) + E_p (\mathcal{R}, \mu, \nu) = \frac{\hbar}{m_e} \mu_{\mathcal{R}, \nu} (\mathcal{R}) \left[ E^C_{\mathcal{R}, \nu} + E^P_{\mathcal{R}, \nu} \right] \]  \quad (4.16)

and

\[ M (\mathcal{R}, \mu, \nu) = M_z (\mathcal{R}, \mu, \nu) + M_p (\mathcal{R}, \mu, \nu) = \frac{\hbar}{m_e} \mu_{\mathcal{R}, \nu} (\mathcal{R}) \left[ M^C_{\mathcal{R}, \nu} + M^P_{\mathcal{R}, \nu} \right] \]  \quad (4.17)

where the terms inside the brackets represent the intrinsic multipole moments of the core, and the multipole moments of the extra-core particle in body coordinates. The quantities on the left-hand side of the equation represent the appropriate multipole operator in laboratory coordinates. It should be noted that these definitions are somewhat arbitrary, as is suggested by the multiplicative factor \( \sqrt{\frac{2k+1}{4\pi}} \) in Equation 4.11, and one must be very careful when comparing these equations with those of other works.

The multipole moments of the particle are given as

\[ E^P_{\mathcal{R}, \nu} = \sqrt{\frac{\hbar^2}{2m_e}} e_p \times \nu \cdot R \chi_{\nu, \nu} (\theta, \phi) \]  \quad (4.18)

and

\[ M^P_{\mathcal{R}, \nu} = M^P_{\mathcal{R}, 0} (\xi) + M^P_{\mathcal{R}, \nu} (\xi) \]

\[ = \sqrt{\frac{\hbar^2}{2m_e}} \mu_N \left[ g_0 \xi + \frac{e_p}{2m_e} g_0 \xi \right] \times \nu \left( \chi_{\nu, \nu} (\theta, \phi) \right) \]  \quad (4.19)

which are identical to those of the independent particle shell model. The constants \( e_p \) and \( \mu_N \) are the proton charge and the nuclear magneton respectively, and the parameters \( g_0 \), \( g_0 \), and \( g_s \) represent the effective charge,
and the orbital and spin gyromagnetic ratios for the extra-core nucleon. If the odd nucleon is a proton, one finds (104, pp. 333-345)

\[ \chi = 1.0 - 0.5 \delta_{s,1} \]
\[ g_s = 0.0 \]
\[ g_s = 5.587 \]

and for a neutron

\[ \chi = -0.5 \delta_{s,1} \]
\[ g_s = 0.0 \]
\[ g_s = -3.826 \]

The electric multipole moment of the core \( E_{\nu,\nu}^C \), can be calculated from Equation 2.63 which is

\[ E_{\nu,\nu}^C = \sqrt{\frac{4\pi}{2\pi \pi^3}} \int d^2 r \, \rho(r) \gamma(r) \tilde{Y}_{\nu,\nu} \left( \hat{r} \right) \]  

(4.22)

In analogy to the Nilsson model, we assume the electric charge of the core to be distributed uniformly out to the surface of the nucleus, so that

\[ \rho(r) = 0 \quad \gamma > R(\theta, \phi) \]
\[ = \frac{3 \pi e}{4 \pi R_0^2} \quad \gamma < R(\theta, \phi) \]

(4.23)

where

\[ R(\theta, \phi) = R_0 \left[ 1 + \sum_{\nu} b_{\nu} \tilde{Y}_{\nu,\nu}^\dagger(\theta, \phi) \right] \]  

(4.24)

Carrying out the integration to first order in the deformation parameters, we find

\[ E_{\nu,\nu}^C = \sqrt{\frac{4\pi}{2\pi \pi^3}} \frac{3 \pi e R_0}{4 \pi} \tilde{\alpha}_\nu (\ell_{\nu,\nu}) \]  

(4.25)
The magnetic multipole operator of Equation 4.19 can be simplified for \( \ell = 1 \) by noting that

\[
\mathbf{A} \cdot \nabla (\mathbf{r} \mathbf{Y}_{1, \mathbf{r}}) = \frac{3}{4 \pi} \mathbf{A} \mathbf{Y}_{1, \mathbf{r}},
\]

where \( \mathbf{A} \) is any vector and \( \mathbf{A} \mathbf{Y} \) is expressed in pseudospherical coordinates.

The magnetic dipole operator of the particle in body coordinates is then simply

\[
\mathbf{M}^b_{1, \mathbf{r}} = \mu \left[ g_s \mathbf{S} + g_e \mathbf{L} \right].
\]

From the discussion given in Section II.E, we see that the intrinsic magnetic dipole moment of the core can be given as

\[
\mathbf{M}^c_{1, \mathbf{r}} = g_c \mu \mathbf{L}.
\]

where \( g_c = \frac{Z}{A} \) is the gyromagnetic ratio of the core, and \( \mathbf{L} \) is the core angular momentum. The total magnetic dipole operator can then be written as

\[
\mathbf{M}^b_{1, \mathbf{r}} = \mu \left[ g_c \mathbf{L} + g_s \mathbf{S} + g_e \mathbf{L} \right].
\]

Using the coupling relations of Equation 3.40, the last equation can be re-written as

\[
\mathbf{M}^b_{1, \mathbf{r}} = \mu \left[ g_c \mathbf{I} + (g_s - g_e) \mathbf{J} + (g_s - g_e) \mathbf{S} \right].
\]

We must also consider higher order magnetic multipole moments of the core. Assuming that the current distributions of the core can be described with some degree of validity by rigid motion of point alpha particles, we find from Equations 2.77 and 2.78 that the intrinsic magnetic multipole
moments of the core can be written as

$$M_{\mathcal{R} \mathcal{V}}^c = \frac{(2J+1)\langle \mathcal{R} \rangle^2}{\langle \mathcal{V} \rangle^2} \mathcal{C}_{\mathcal{R}, \mathcal{V}}(\mathcal{R}, \mathcal{V}) \langle \mathcal{R}, \mathcal{V} \rangle$$

(4.31)

where the coefficients

$$\mathcal{C}_{\mathcal{R}, \mathcal{V}}(\mathcal{R}, \mathcal{V}) = \mathcal{C}(\mathcal{R}, \mathcal{V})$$

(4.32)

are constants which depend explicitly on the size and shape of the \(\alpha\)-structure.

3. Calculating the reduced matrix elements

The matrix element involving the electric moment of the core can be readily evaluated by using Equations 4.14, 4.16, and C12 as follows:

$$\langle N'I's'j'm'; K'IM'| E_c(\mathcal{R}, \mathcal{V}) | NX'sjm; KIM \rangle$$

$$= E_{\mathcal{R} \mathcal{V}}^c \mathcal{S}_{\mathcal{R} \mathcal{V}} \mathcal{S}_{ss} \mathcal{S}_{dd} \mathcal{S}_{mm'}$$

(4.33)

The complexity of Equations 4.31 and 4.32 offers little incentive for attempting to evaluate general matrix elements of \(\mathcal{H}^c\). Therefore, we shall ignore magnetic core contributions except for M1 transitions. The necessary matrix element for this operator can be easily evaluated by using Equation D7, and is

$$\langle N'I's'j'm'; K'IM'| g_e I_{\mu \nu} | NX'sjm; KIM \rangle$$

$$= g_e \langle I_{\mu \nu} \rangle \mathcal{S}_{\mathcal{R} \mathcal{V}} \mathcal{S}_{ss} \mathcal{S}_{dd} \mathcal{S}_{mm'}$$

(4.34)

Fortunately, the pretermission of core contributions to M2 and M3 transitions
is not too serious in the present work, because very few experimental transitions of this type will be encountered for the A=13 nuclei that we will consider in Section E.

All of the matrix elements of the extra-core particle operator, \( \lambda_p(k,\mu) \), can be separated into collective and particle terms as follows:

\[
\langle N' e' s' f' m' ; k' I' m' | \lambda_p(k,\mu) | N e s f m; k I m \rangle
\]

\[
= \sqrt{\frac{2I+1}{4\pi}} \sum \langle k' I' m' | D^{R}_{N' N} (A) | k I m \rangle \langle N' e' s' f' m' | \lambda^{p}_{N' N} | N e s f m \rangle.
\]

The first term can be evaluated by Equation C12, but the last term requires extensive Racah algebra. We shall consider first the electric contribution and rewrite the particle term (via Equation 4.18) as

\[
\langle N' e' s' f' m' | E^p_{N' N} | N e s f m \rangle
\]

\[
= \sqrt{\frac{4\pi}{2^{2A+1}}} e_p \alpha \langle N' e' s' f' m' | \lambda^{p}_{N' N} | N e s f m \rangle.
\]

This matrix element can be solved using the decoupling relation of Equation C1, Equation C17, the recoupling formula of Equation C26, and the identity of Equation C27. The final result is

\[
\langle N' e' s' f' m' | E^p_{N' N} | N e s f m \rangle = \frac{[1 + (-)^{s+2'+R}]}{2} e_p \alpha (-)^{s+m'}
\]

\[
\times \langle N' e' | \lambda^{R}_{N N} | N e \rangle \sqrt{(2s+1)(2s'+1)} \left( \begin{array}{c} \frac{A}{2} \frac{A}{2} \frac{A}{2} \frac{A}{2} \end{array} \right) \left( \begin{array}{c} \frac{R}{2} \frac{R}{2} \frac{R}{2} \frac{R}{2} \end{array} \right) \left( \frac{m}{2} \frac{m}{2} \frac{m}{2} \frac{m}{2} \right).
\]

The magnetic matrix elements are much harder to evaluate, and one must consider the spin and orbital parts separately. The matrix element arising from the spin of the particle is
\[ \langle \mathcal{N}'\mathcal{E}'\mathcal{s}'\mathcal{j}'\mathcal{m}'| \mathcal{M}^{P}_{\mathcal{R}_{\mathcal{N}}}(\mathcal{J})| \mathcal{N}\mathcal{E}\mathcal{s}\mathcal{j}\mathcal{m}\rangle = \]
\[ = \sqrt{\frac{4\pi}{2\mathcal{R}+1}} \mathcal{N}_{\mathcal{E}} \langle \mathcal{N}'\mathcal{E}'\mathcal{s}'\mathcal{j}'\mathcal{m}'| \mathcal{M}^{P}_{\mathcal{R}_{\mathcal{N}}}(\mathcal{J})| \mathcal{N}\mathcal{E}\mathcal{s}\mathcal{j}\mathcal{m}\rangle , \]

which can be evaluated from the decoupling relations of Equation C1, the identity of Equation C17, and the coupling relation of Equation C28. The result is

\[ \langle \mathcal{N}'\mathcal{E}'\mathcal{s}'\mathcal{j}'\mathcal{m}'| \mathcal{M}^{P}_{\mathcal{R}_{\mathcal{N}}}(\mathcal{J})| \mathcal{N}\mathcal{E}\mathcal{s}\mathcal{j}\mathcal{m}\rangle = (-)^{\mathcal{j}'+\mathcal{j}'-\mathcal{m}'} \delta_{\mathcal{s}\mathcal{s}'} \langle \mathcal{N}'\mathcal{E}'| \mathcal{N}\mathcal{E}^{*-1}\mathcal{N}\mathcal{E}\rangle \mathcal{N}_{\mathcal{E}} X \left( \begin{array}{ccc}
\mathcal{j}' & \mathcal{j} & \mathcal{R} \\
m & m' & \mathcal{R} - m' \\
0 & 0 & 0
\end{array} \right) \sqrt{5(5+1)(2\mathcal{R}+1)(2\mathcal{R}_n-1)(2\mathcal{R}_n+1)(2\mathcal{j}'+1)(2\mathcal{j}'+1)} \]

\[ \times \left( \begin{array}{ccc}
\mathcal{R} & \mathcal{R} & \mathcal{R} - 1 \\
\mathcal{j} & \mathcal{j} & \mathcal{R} - \mathcal{m}' \\
\mathcal{s} & \mathcal{s}' & 1
\end{array} \right) \left( \begin{array}{ccc}
\mathcal{j}' & \mathcal{j} & \mathcal{R} \\
\mathcal{R} & \mathcal{R} & \mathcal{R} - m' \\
0 & 0 & 0
\end{array} \right) \right) . \] (4.39)

Fortunately, the above expression using Equations C27 and C28, and noting that the explicit expression for one of the 6-J symbols that arises in the calculation is (109, p. 16)

\[ \left\{ \mathcal{R} \atop \mathcal{R} \atop \frac{1}{2} \atop \frac{1}{2} \right\} = \frac{1}{\mathcal{G}\mathcal{R}} . \] (4.40)

The final result is

\[ \langle \mathcal{N}'\mathcal{E}'\mathcal{s}'\mathcal{j}'\mathcal{m}'| \mathcal{M}^{P}_{\mathcal{R}_{\mathcal{N}}}(\mathcal{J})| \mathcal{N}\mathcal{E}\mathcal{s}\mathcal{j}\mathcal{m}\rangle = (-)^{\mathcal{j}'+\mathcal{j}'-\mathcal{m}'} \delta_{\mathcal{s}\mathcal{s}'} \frac{[1+(\cdot)^{\mathcal{j}'+\mathcal{j}'+\mathcal{R} - 1}]}{2} \]

\[ \times \mathcal{N}_{\mathcal{E}} \mathcal{N}_{\mathcal{E}} \sqrt{\frac{(2\mathcal{R}+1)(2\mathcal{R}_n+1)(2\mathcal{j}'+1)}{4\pi}} \langle \mathcal{N}'\mathcal{E}'| \mathcal{N}\mathcal{E}^{*-1}\mathcal{N}\mathcal{E}\rangle \left( \begin{array}{ccc}
\mathcal{j}' & \mathcal{j} & \mathcal{R} \\
\mathcal{R} & \mathcal{R} & \mathcal{R} - m' \\
0 & 0 & 0
\end{array} \right) \left( \begin{array}{ccc}
\mathcal{j}' & \mathcal{j} & \mathcal{R} \\
\mathcal{R} & \mathcal{R} & \mathcal{R} - m' \\
0 & 0 & 0
\end{array} \right) \right) . \] (4.41)
The matrix element arising from the orbital part of the particle is

\[
\langle N' e' s' j' m' | M_{\mathcal{R}, \mathcal{V}}^P (\xi) | N e s j m \rangle = \sqrt{\frac{4\pi}{2\mathcal{R}+1}} \ g_{e\mathcal{R}N} \langle N' e' s' j' m' | \mathcal{R} \cdot \mathcal{V} [\mathcal{R}_{\mathcal{R}, \mathcal{V}}\mathcal{V}(v', q')] | N e s j m \rangle ,
\]

and can be evaluated by the decoupling relation of Equation C1, the identity of Equation C17, and two separate applications of the recoupling relation of Equation C26. The result is

\[
\langle N' e' s' j' m' | M_{\mathcal{R}, \mathcal{V}}^P (\xi) | N e s j m \rangle = (-1)^{s-m'} \langle N' e' | \mathcal{R}^{-1} | N e \rangle \ g_{e\mathcal{R}N} \\
\times \frac{1}{\sqrt{\left(2_{\mathcal{R}+1}(2_{\mathcal{R}+1})(2_{\mathcal{R}+1})(2_{\mathcal{R}+1})(2_{\mathcal{R}+1})(2_{\mathcal{R}+1})(2_{\mathcal{R}+1})(2_{\mathcal{R}+1})(2_{\mathcal{R}+1})\right)}}
\times \left( \begin{array}{c} \mathcal{R} \mathcal{V} \\ \mathcal{R} \mathcal{V} \mathcal{V} \end{array} \right) \left( \begin{array}{ccc} s' & j' & m' \\ 0 & 0 & 0 \end{array} \right) \left( \begin{array}{ccc} s & \mathcal{R} & j \\ 0 & 0 & 0 \end{array} \right) \\
\times \left( \begin{array}{c} s' \mathcal{R} j' \\ s \mathcal{R} j \\ 0 \end{array} \right) \\
\times \left( \begin{array}{c} j' \\ j \\ 0 \end{array} \right) .
\]

From Equations 4.29 and 4.30, we see that the particle matrix elements for an M1 transition involve only the operators $s$, $\mathcal{R}$, and $j$. The necessary matrix elements can be readily evaluated and are

\[
\langle N' e' s' j' m' | S_\mathcal{V} | N e s j m \rangle = S_{N'N} \ S_{e'e} \ S_{s's} \sqrt{\frac{3(2_{\mathcal{R}+1})(2_{\mathcal{R}+1})}{2}}
\times (-1)^{s+s'+m'+j'},
\]

\[
\times \left( \begin{array}{ccc} s & j & m' \\ 0 & 0 & 0 \end{array} \right) \left( \begin{array}{ccc} s' & j' & m' \\ 0 & 0 & 0 \end{array} \right) \left( \begin{array}{ccc} s & j \mathcal{R} & s' \mathcal{R} j' \\ 0 & 0 & 0 \end{array} \right) \\
\times \left( \begin{array}{c} j' \mathcal{R} \\ j \mathcal{R} \end{array} \right) .
\]

and

\[
\langle N' e' s' j' m' | j_\mathcal{V} | N e s j m \rangle = S_{N'N} \ S_{e'e} \ S_{s's} \ (-1)^{s+m'-j'}
\times \sqrt{\frac{3(2_{\mathcal{R}+1})(2_{\mathcal{R}+1})(2_{\mathcal{R}+1})(2_{\mathcal{R}+1})}{2}}
\times \left( \begin{array}{ccc} s & j & m' \\ 0 & 0 & 0 \end{array} \right) \left( \begin{array}{ccc} s' & j' & m' \\ 0 & 0 & 0 \end{array} \right) \\
\times \left( \begin{array}{c} j' \mathcal{R} \\ j \mathcal{R} \end{array} \right) .
\]

and

\[
\langle N' e' s' j' m' | \mathcal{R}_\mathcal{V} | N e s j m \rangle = S_{N'N} \ S_{e'e} \ S_{s's} \ S_{\mathcal{R}\mathcal{R}'}
\times \sqrt{\frac{3(2_{\mathcal{R}+1})(2_{\mathcal{R}+1})}{2}}
\times \left( \begin{array}{ccc} s & j & m' \\ 0 & 0 & 0 \end{array} \right) \left( \begin{array}{ccc} s' & j' & m' \\ 0 & 0 & 0 \end{array} \right) \\
\times \left( \begin{array}{c} j' \mathcal{R} \\ j \mathcal{R} \end{array} \right) .
\]
In order to evaluate the matrix element of the total particle operator, \( \lambda_p(R, \mathbf{\mu}) \), we must now combine Equation 4.35 with the appropriate particle matrix element. However, in doing this, we shall make use of the Wigner-Eckart theorem which for the present case is

\[
\langle N'l'e's'd'm' ; \mu_l' \mu_m' | \lambda_p(R, \mathbf{\mu}) | N'e's'd'm ; \mu_l \mu_m \rangle
\]

\[
= (-)^{I'-I} \left( \begin{array}{c} I' \\mu_l' \\ -\mu_m' \end{array} \right) \langle N'l'e's'd'm' ; \mu_l' \mu_m' | N'e's'd'm ; \mu_l \mu_m \rangle
\]

and present the results in terms of reduced matrix elements. The reduced matrix element of the electric part of the particle is

\[
\langle N'l'e's'd'm' ; \mu_l' \mu_m' | \lambda_p(R, \mathbf{\mu}) | N'e's'd'm ; \mu_l \mu_m \rangle = \delta_{s's'} (-)^{s+m'+s'+m} \frac{1}{2} \left( \begin{array}{c} R' \\mu_l' \\ R \\mu_l \end{array} \right)
\]

\[
\times \sqrt{(2I'+1)(2I'+1)(2\frac{1}{2}+1)(2\frac{1}{2}+1)} \langle N'l'e' | \mathbf{\mu} | N'e \rangle \left( \begin{array}{c} \mu_l' \\mu_l \\ -\mu_m' \mu_m \end{array} \right)
\]

while the magnetic contribution can be expressed as

\[
\langle N'l'e's'd'm' ; \mu_l' \mu_m' | \lambda_p(R, \mathbf{\mu}) | N'e's'd'm ; \mu_l \mu_m \rangle
\]

\[
= \langle N'l'e's'd'm' ; \mu_l' \mu_m' | \lambda_p(R, \mathbf{\mu}) + \lambda_p(R, \mathbf{\mu}) | N'e's'd'm ; \mu_l \mu_m \rangle
\]

where

\[
\langle N'l'e's'd'm' ; \mu_l' \mu_m' | \lambda_p(R, \mathbf{\mu}) | N'e's'd'm ; \mu_l \mu_m \rangle = (-)^{I'+I'+s+m'+m'}
\]

\[
\times \frac{1+(-1)^{I'+s'+\frac{3}{2}-I}}{2} \sqrt{(2I'+1)(2I'+1)(2\frac{1}{2}+1)(2\frac{1}{2}+1)} \langle N'l'e' | \mathbf{\mu} | N'e \rangle \left( \begin{array}{c} \mu_l' \\mu_l \\ -\mu_m' \mu_m \end{array} \right)
\]

and

\[
\langle N'l'e's'd'm' ; \mu_l' \mu_m' | \lambda_p(R, \mathbf{\mu}) | N'e's'd'm ; \mu_l \mu_m \rangle = (-)^{I'+I'+s+m'} \langle N'l'e' | \mathbf{\mu} | N'e \rangle \frac{2}{2} \times \sqrt{(2I'+1)(2I'+1)(2\frac{1}{2}+1)(2\frac{1}{2}+1)} \langle N'l'e' | \mathbf{\mu} | N'e \rangle \left( \begin{array}{c} \mu_l' \\mu_l \\ -\mu_m' \mu_m \end{array} \right)
\]
For magnetic dipole moments, the necessary reduced matrix elements for the
particle spins are

\[ < \nu' s' \tilde{d}' m'; \nu' \tilde{d}' m; \nu \tilde{d} m; \nu \tilde{d} m; \nu' \tilde{d}' m' > = (-)^{I' - K' + s' + m' + \tilde{d}' + \tilde{d}} S_{\nu \nu'} S_{\tilde{d} \tilde{d}'} S_{s m} \]  

\[ \times \frac{(2 \tilde{d} + 1)(2 \tilde{d}' + 1)(2 \tilde{d}' + 1)(2 \tilde{d}')}{2} \]

\[ \times \left\{ \begin{array}{c}
\tilde{d}' \tilde{d}' \\
\nu' \nu \end{array} \right\} \left\{ \begin{array}{c}
\tilde{d} \tilde{d} \\
m m' \end{array} \right\} \]  

(4.52)

\[ < \nu' s' \tilde{d}' m'; \nu' \tilde{d}' m; \nu \tilde{d} m; \nu \tilde{d} m; \nu' \tilde{d}' m' > = (-)^{s' + \tilde{d}' + \tilde{d} + m' + \tilde{d}} S_{\nu \nu'} S_{\tilde{d} \tilde{d}'} S_{s m} \]

\[ \times \frac{(2 \tilde{d} + 1)(2 \tilde{d}' + 1)(2 \tilde{d}' + 1)(2 \tilde{d}')}{2} \]

\[ \times \left\{ \begin{array}{c}
\tilde{d}' \tilde{d}' \\
\nu' \nu \end{array} \right\} \left\{ \begin{array}{c}
\tilde{d} \tilde{d} \\
m m' \end{array} \right\} \]  

(4.53)

and

\[ < \nu' s' \tilde{d}' m'; \nu' \tilde{d}' m; \nu \tilde{d} m; \nu \tilde{d} m; \nu' \tilde{d}' m' > = (-)^{I' + \tilde{d}' + m' + \tilde{d} + s} S_{\nu \nu'} S_{\tilde{d} \tilde{d}'} S_{s m} S_{\tilde{d} \tilde{d}'} \]

\[ \times \frac{(2 \tilde{d} + 1)(2 \tilde{d}' + 1)(2 \tilde{d}' + 1)(2 \tilde{d}')}{2} \]

\[ \times \left\{ \begin{array}{c}
\tilde{d}' \tilde{d}' \\
\nu' \nu \end{array} \right\} \left\{ \begin{array}{c}
\tilde{d} \tilde{d} \\
m m' \end{array} \right\} \]  

(4.54)

while the reduced matrix element of the total spin \( I \) is simply

\[ < \nu' s' \tilde{d}' m'; \nu' \tilde{d}' m; \nu \tilde{d} m; \nu \tilde{d} m; \nu' \tilde{d}' m' > = S_{\nu \nu'} S_{\tilde{d} \tilde{d}'} S_{s m} \]  

(4.55)

Finally, we present the reduced matrix element caused by the intrinsic electro­meric multipole moment of the core. From Equation 4.33 we find

\[ < \nu' s' \tilde{d}' m'; \nu' \tilde{d}' m; \nu \tilde{d} m; \nu \tilde{d} m; \nu' \tilde{d}' m' > = (-)^{I' - K'} \]

\[ \times \frac{1}{4 \pi} \frac{\tilde{d} \tilde{d}'}{s m} \sqrt{(2 \tilde{d} + 1)(2 \tilde{d}' + 1)} \]  

(4.56)

The transitions cannot be developed further until we consider the exact form
of the final wavefunction such as given in Equation 4.7 or 4.8. This form
depends on the symmetry of the structure, and so such calculations must be
done individually for each nucleus.
D. Brief Review of the Mass A=9 System

In our development of the UAP model, we have not attempted to construct individual alpha clusters within the deformed core, but have merely assumed that such a structure exists, and that the resultant potential between the core and extra-core nucleon can be approximated by Equation 4.4. Consequently, if our model were applied to the mass A=9 system, the results would be identical to that of the Nilsson model, because the $^8$Be dumbbell core has $D_4h$ symmetry.

Unfortunately, the experimental data for $^9$Be is quite scarce and practically nonexistent for the mirror nucleus $^9$B. In fact, all nuclear models predict $1/2^-$ and $3/2^-$ levels below 6 MeV (110), and neither of these states has yet been observed experimentally. Also, up until four years ago the experimental static quadrupole moment for the $3/2^-$ ground state of $^9$Be was incorrectly determined from several different measurements of the hyperfine structure to be $Q_{3/2}^- = 2.9 \text{ fm}^2$ (111,112). The error did not come from the measuring of the hyperfine splitting, but resulted because of the difficulties involved in computing an accurate value for the gradient of the atomic electric field at the nucleus. The value of $2.9 \text{ fm}^2$ was found to be in excellent agreement with the shell model calculations (113), but too small by a factor of two from the predictions of collective models (31,32,114,115).

Then, in 1967 the electric field gradient was recalculated and found to be smaller than previously assumed (116). The revised experimental quadrupole moment is now $Q_{3/2}^- = 5.26 \pm 0.30 \text{ fm}^2$ which is in good agreement with the predictions of various collective models.

Several attempts have been made within the past fifteen years to explain the properties of $^9$Be using modified $\alpha$-particle calculations that are
somewhat different from those of the Nilsson model. The results are quite successful, and an accurate value for the separation distance between the two alpha particles can be obtained from this work. Therefore, a brief review of these calculations should be included in the present work. In 1958, Blair and Henley (117) proposed a "strongly-coupled $\alpha$-particle model" for $^{9}$Be by assuming the Hamiltonian and wavefunctions to be of the form

$$ H = A \mathbf{L} \cdot \mathbf{L} + V(d) $$

and

$$ \langle \lambda^\prime \lambda \mathbf{m} \lambda \mathbf{m} | \mathbf{M} \mathbf{M} \rangle = \frac{2 \pi}{\sqrt{\lambda ! \lambda !}} R(d) \left[ D_{\lambda \lambda}^{\mathbf{m}}(\alpha) \Phi_{\lambda \mathbf{m}}^{(\alpha)} + (-)^{\lambda} D_{\lambda \lambda}^{\mathbf{m}}(\alpha) \Phi_{\lambda \mathbf{m}}^{(-\alpha)} \right], $$

where $R(d)$ is the vibrational function of the two alphas with $d$ being the inter-alpha distance, and $\Phi_{\lambda \mathbf{m}}^{(\alpha)}(r)$ the neutron wavefunction referred to the body coordinate system. As in the Nilsson model, this model is capable of predicting the experimental $3/2^-(0.0 \text{ MeV})$, $5/2^-(2.43 \text{ MeV})$, and $7/2^-(6.76 \text{ MeV})$ levels as rotational states built on a deformed $K=3/2^-$ band with a rotational parameter $A_I=0.48 \text{ MeV}$. Using this value, they then treated the core as a rigid rotor of point $\alpha$-particles and found the alpha separation to be $d=4.6 \text{ fm}$. (If one includes the finite rms radius of the alpha particle in the calculations, the separation distance is reduced to $d=3.8 \text{ fm}$.) They also estimated the separation distance by developing an approximate theory for the alpha scattering cross-sections. By comparing their theory to the inelastic scattering data for the excited $5/2^-$ state, they found best agreement with $d=5.4 \text{ fm}$. This large value can be attributed partly to centripetal distortion and also to the quite drastic approximations that went into the theory. More recently, at least two other authors have used these wavefunctions to calculate the elastic electron scattering cross-section curve
using the same method as derived in Section II E. The best agreement with experiment is obtained with $d=3.8$ fm which corresponds to a static quadrupole moment of $Q_{3/2}^-=5.8$ fm$^2$ (31,32); this value is in good agreement with the most recent value determined from the hyperfine splitting as noted earlier.

One other type of $\alpha$-particle was formulated by Kunz (118) in 1960 who assumed a realistic Hamiltonian for $^9$Be of the form

$$H = K + V(r,c) + H(c),$$

where $K$ is the neutron energy, $V(r,c)$ is the interaction of the neutron with the $\alpha$-core, and $H(c)$ is the Hamiltonian of the core. A few years later, the model was improved by the addition of a phenomenological $\alpha-\alpha$ interaction to the core Hamiltonian (119). The energy levels were then found by variational techniques with no free parameters. Besides obtaining fair agreement with the position of the experimental levels, the static quadrupole moment was found to be 4.6 fm$^2$, and the magnetic moment $\mu=-1.21\mu_N$, both of which are close to the experimental values (120). Such realistic calculations as these are not justified for higher $A=4N+1$ nuclei because the alpha clusters in this theory are considered as stable entities within the nucleus. Our previous work on the $A=4N$ nuclei in Chapter II indicates that this approximation is most likely not valid for $A \geq 12$.

E. $D_{3h}$ Symmetry for the Mass $A=13$ Nuclei

1. Constructing the basis functions

Perhaps the easiest way constructing a set of basis vectors for $D_{3h}$ is to consider the analogous spinors for one of its cover groups, $D_{6h}$. In the
last chapter, it was shown that the basis states for $D_{\omega h}$ could be written as

$$
\begin{pmatrix}
\Phi_1 \\
\Phi_2
\end{pmatrix} \sim \begin{pmatrix}
|\frac{1}{2}, m \rangle \\
-|\frac{1}{2}, m \rangle
\end{pmatrix}.
$$

These spinors will automatically be basis functions for one of the three IR's of $D_{3h}$, and the appropriate $D_{3h}$ IR label for each spinor can be found from Table 4.4. By arbitrarily choosing one of the three 2-fold symmetry axes of the triangular-shaped core to coincide with the body-fixed $x$ axis, we find from Equation 3.36 that all three double-valued IR's of $D_{3h}$ will have the same matrix representation for $C_{2x}$, namely $\begin{pmatrix}
0 & i \\
i & 0
\end{pmatrix}$. The trace of this matrix is zero, which agrees with the corresponding three characters of the $D_{3h}$ character table (Table 4.2).

The above matrix for $C_{2x}$ gives only the relative phase between the two components of the spinor, and therefore does not uniquely determine the basis functions. The final construction, however, can be easily accomplished by arbitrarily choosing an exact form for one of the many possible basis states of each IR. We shall therefore simply construct the three "defining" basis spinors to be

$$
\begin{pmatrix}
|\frac{1}{2}, m \rangle \\
-|\frac{1}{2}, m \rangle
\end{pmatrix} = \begin{pmatrix}
|\frac{1}{2}, \frac{1}{2}, + \rangle \\
-|\frac{1}{2}, -\frac{1}{2}, + \rangle
\end{pmatrix}
$$

for $\Gamma_1$,

$$
\begin{pmatrix}
|\frac{1}{2}, m \rangle \\
-|\frac{1}{2} + \frac{1}{2}, m \rangle
\end{pmatrix} = \begin{pmatrix}
|\frac{1}{2}, \frac{1}{2}, - \rangle \\
-|\frac{1}{2}, -\frac{1}{2}, - \rangle
\end{pmatrix}
$$

for $\Gamma_2$, and
It should be noticed that the defining relations were performed on the spinors with the smallest value of \( j \) and \( |m| \) for each IR, and that the above three relations are consistent with the relative phase given in Equation 4.60. We now employ a relation from group theory which states that if \( H \) is invariant under all operations of a group, and if \( \psi_i \) is a basis function of the \( i \)th row in the \( \chi \)th IR, then (30, p. 166)

\[
\langle \phi_{a}' | H | \psi_{a} \rangle = \epsilon \sigma_{a} \sigma_{a}' \sigma_{z} \sigma_{z}'
\]

That is, the matrix element can be nonzero only if the wavefunctions are basis states of the same row of the IR, as well as the same IR. A careful analysis of the most general particle Hamiltonian one can construct having \( D_{3h} \) symmetry (c.f. Equation 4.5) shows that the matrix element \( \langle \phi_{a}' | H | \psi_{a} \rangle \) can be nonzero only if (a) \( |m' - m| \) is an odd multiple of three and \( \pi \pi' = -1 \), or (b) \( |m' - m| \) is an even multiple of three and \( \pi \pi' = +1 \). Using this restriction along with the defining basis functions of Equations 4.61, 4.62, and 4.63, we can readily tabulate the particle wavefunctions as shown in Table 4.6. Only the parity and magnetic quantum numbers of the top component of each spinor are shown. Any additional information that could be given would be redundant because all \( j \geq |m| \) are allowed for each IR, and the bottom component of the spinor is always given by \( (-)^{j+1/2} |j, -m, \pi \rangle \). Using the information of Table 4.6, we can now classify the wavefunctions of the spherical harmonic oscillator as basis functions of the \( D_{3h} \) point group. This classification can be readily accomplished if we remember that parity
Table 4.6. The top component of the spinor belonging to the $\Gamma_i$ IR can have only the quantum numbers $m$ and $\pi$ given below. All $j > |m|$ are allowed for each $m$.

<table>
<thead>
<tr>
<th>$\Gamma_i$</th>
<th>$m$</th>
<th>1/2</th>
<th>-5/2</th>
<th>7/2</th>
<th>-11/2</th>
<th>13/2</th>
<th>-17/2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\pi$</td>
<td>+</td>
<td>-</td>
<td>-</td>
<td>+</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>$\pi$</td>
<td>-</td>
<td>+</td>
<td>+</td>
<td>-</td>
<td>-</td>
<td>+</td>
</tr>
<tr>
<td>3</td>
<td>$\pi$</td>
<td>+</td>
<td>-</td>
<td>+</td>
<td>-</td>
<td>+</td>
<td>-</td>
</tr>
</tbody>
</table>
for these wavefunctions goes as (-)\(^n\). The results are given in Table 4.7. Again, only the quantum numbers of the top component of each spinor are given for each eigenstate. The diagonalized particle wavefunctions for a particular set of deformation coefficients can now be given as

\[ |\Gamma_1,1\rangle = \sum_{(\Lambda \Sigma \Lambda \Sigma \Sigma \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \Delta \D
Table 4.7. The allowed quantum numbers for the top component of the spinor basis functions of the spherical harmonic oscillator, $|N, \ell, s, j, m\rangle$, are presented for each IR of $D_{3h}$ up through the $n=5$ oscillator shell. Only the states above the dashed line were included in most of the calculations.

<table>
<thead>
<tr>
<th>Basis function number</th>
<th>$\ell_1$</th>
<th>$\ell_2$</th>
<th>$\ell_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0 0 1/2 1/2</td>
<td>1 1 3/2 1/2</td>
<td>1 1 3/2 -3/2</td>
</tr>
<tr>
<td>2</td>
<td>2 2 5/2 1/2</td>
<td>1 1 1/2 1/2</td>
<td>2 2 5/2 3/2</td>
</tr>
<tr>
<td>3</td>
<td>2 2 3/2 1/2</td>
<td>2 2 5/2 -5/2</td>
<td>2 2 3/2 3/2</td>
</tr>
<tr>
<td>4</td>
<td>2 0 1/2 1/2</td>
<td>3 3 7/2 1/2</td>
<td>3 3 7/2 -3/2</td>
</tr>
<tr>
<td>5</td>
<td>3 3 7/2 7/2</td>
<td>3 3 5/2 1/2</td>
<td>3 3 5/2 -3/2</td>
</tr>
<tr>
<td>6</td>
<td>3 3 7/2 -5/2</td>
<td>3 1 3/2 1/2</td>
<td>3 1 3/2 -3/2</td>
</tr>
<tr>
<td>7</td>
<td>3 3 5/2 -5/2</td>
<td>3 1 1/2 1/2</td>
<td>4 4 9/2 3/2</td>
</tr>
<tr>
<td>8</td>
<td>4 4 9/2 1/2</td>
<td>4 4 9/2 -5/2</td>
<td>4 4 9/2 -9/2</td>
</tr>
<tr>
<td>9</td>
<td>4 4 7/2 1/2</td>
<td>4 4 9/2 7/2</td>
<td>4 4 7/2 3/2</td>
</tr>
<tr>
<td>10</td>
<td>4 2 5/2 1/2</td>
<td>4 4 7/2 -5/2</td>
<td>4 2 5/2 3/2</td>
</tr>
<tr>
<td>11</td>
<td>4 2 3/2 1/2</td>
<td>4 4 7/2 7/2</td>
<td>4 2 3/2 3/2</td>
</tr>
<tr>
<td>12</td>
<td>4 0 1/2 1/2</td>
<td>4 2 5/2 -5/2</td>
<td>5 5 11/2 -3/2</td>
</tr>
<tr>
<td>13</td>
<td>5 5 11/2 -5/2</td>
<td>5 5 11/2 1/2</td>
<td>5 5 11/2 9/2</td>
</tr>
<tr>
<td>14</td>
<td>5 5 11/2 7/2</td>
<td>5 5 11/2 -11/2</td>
<td>5 5 9/2 -3/2</td>
</tr>
<tr>
<td>15</td>
<td>5 5 9/2 -5/2</td>
<td>5 5 9/2 1/2</td>
<td>5 5 9/2 9/2</td>
</tr>
<tr>
<td>16</td>
<td>5 5 9/2 7/2</td>
<td>5 3 7/2 1/2</td>
<td>5 3 7/2 -3/2</td>
</tr>
<tr>
<td>17</td>
<td>5 3 7/2 -5/2</td>
<td>5 3 5/2 1/2</td>
<td>5 3 5/2 5/2</td>
</tr>
<tr>
<td>18</td>
<td>5 3 7/2 7/2</td>
<td>5 3 3/2 1/2</td>
<td>5 1 3/2 -3/2</td>
</tr>
<tr>
<td>19</td>
<td>5 3 5/2 -5/2</td>
<td>5 1 1/2 1/2</td>
<td>5 1 1/2 1/2</td>
</tr>
</tbody>
</table>
Figure 4.1. Energy levels of the particle Hamiltonian plotted as a function of the deformation parameter $\beta_3$. The diagonalization was carried out among all basis functions below the (a) $N=3$ and (b) $N=5$ oscillator shells. The other parameters used are $\beta_2=-0.4, \chi=0.075, \text{and } \mu=0$, and are chosen so that when $\beta_3=0.0$, the levels degenerate to those of Figure 3.1 (with $\beta_2=0.4$).
particle can occupy. An examination of the final energy levels plotted for a typical set of parameters (as presented in Figure 3.3) shows that this rearranging of particle states will alter the spins and energies of the lowest-lying theoretical states. It will be shown later that the only requirement needed for obtaining favorable agreement between the experimental and theoretical energy levels is that the second \( I_1 \) particle level must be about 0.10\( \hbar \omega \) above the second \( I_2 \) level without having any additional particle levels in the same energy region. After several computer runs, it was found that the Nilsson model alone could not account for this level spacing of the particle levels, and for this one reason, the UAP model was found to give a definite improvement over the Nilsson model for the energy spectra of the \( A=13 \) nuclei (as will be shown shortly). This result is somewhat surprising, since before the calculations were made we expected that the main improvement offered by the UAP model would be caused from the additional energy levels which arise due to the reduction in core symmetry (as indicated by the dotted lines in Figure 3.3). However, these additional levels were found to be of secondary importance when comparisons with experiment were made.

Figure 4.1b shows the same ten particle states as before, except now the diagonalization is performed among all spherical basis states up through the \( N=5 \) oscillator shell. From Table 4.7 we find that the matrices will now include up to 19 basis states. Notice that there is considerable variance in the energy levels of the two graphs, particularly at large values of \( \beta_3 \). However, after considerable calculation, it was found that the final agreement with experiment was not noticeably improved when this expanded basis was used. Therefore, our present calculations will include
only the smaller basis. It will soon be shown that such an approximation allows the computations of the final energy levels to be carried out in a much shorter time.

By arguments similar to those used in obtaining Equation 3.50, we can show that the final Hamiltonian must be diagonalized among coupled basis functions of the form

\[ |\Gamma_i; \alpha \rangle = \sqrt{\frac{1}{2}} \sum_{\chi \sigma \gamma} C_{\chi \sigma \gamma}^\alpha |\chi \sigma \gamma \rangle \]

where \( \alpha \) is the \( \alpha \)th energy level with the IR table \( \Gamma_i \). Again, as explained for the symmetric rotor, we limit the particle eigenstates, \( \Gamma_i \), allowed in the final diagonalization to be those that are accessible to the extra-core nucleon. The quantum numbers \( IK \) that are allowed in Equation 4.63 for a particular \( \Gamma_i \) are again easily found by group theory. For the present, we merely state that the above wavefunction has the correct symmetry whenever the quantum numbers \( K \) and \( \Pi \) have the same values as do \( m \) and \( \eta \) in Table 4.6.

2. Matrix elements of the total Hamiltonian

Since the \( ^{12}\text{C} \) core is a symmetric top, we can write the total Hamiltonian as

\[ H = A_1 L^2 + L_2 (A_3 - A_1) + H_P \]

However, in Chapter II it was found that the two rotational parameters for the collective Hamiltonian of \( ^{12}\text{C} \) had to be nearly equal in order to fit the observed spectrum (as was shown in Table 2.9). If we assume this equality holds for the mass \( A = 13 \) nuclei, we can ignore the second term and write the Hamiltonian as
\[ H = H_c + H_p \quad , \]  

(4.69)

where

\[ H_c = A_i \mathbf{L}^2 = A_i (\mathbf{I}^2 + \mathbf{r}^2 - 2 \mathbf{I}_{xy} \mathbf{r}_{xy}) - 2 A_i (\mathbf{I}_{xy} \mathbf{r}_{xy} + \mathbf{I}_{yz} \mathbf{r}_{yz}) \quad . \]  

(4.70)

This approximation does not simplify the calculations considerably, but it does introduce one less parameter which is desirable. By introducing the quantities

\[ \mathbf{I}_{\pm 1} = \mp \sqrt{\frac{1}{2}} (\mathbf{I}_x \pm i \mathbf{I}_y) \]

and

\[ \mathbf{I}_{\pm 1} = \mp \sqrt{\frac{1}{2}} (\mathbf{I}_x \pm i \mathbf{I}_y) \quad , \]

(4.71)

and defining a dimensionless variable \( \alpha_i \) as

\[ \alpha_i = \frac{A_i}{\hbar \omega} \quad , \]

(4.72)

we can rewrite Equation 4.70 as

\[ H_c = \hbar \omega \alpha_i \left[ (\mathbf{I}^2 + \mathbf{r}^2 - 2 \mathbf{I}_{xy} \mathbf{r}_{xy}) + 2 (\mathbf{I}_x \mathbf{r}_{xy} + \mathbf{I}_y \mathbf{r}_{yz}) \right] \quad . \]  

(4.73)

Since the particle Hamiltonian has already been diagonalized, the matrix elements of the second term in Equation 4.69 may be written as

\[ \langle \mathbf{r}_i' \mathbf{r}_i ; \mathbf{r}_i' \mathbf{r}_m | H_p | \mathbf{r}_i \mathbf{r}_j \mathbf{r}_k \mathbf{r}_m \rangle = s_{\mathbf{r}_i \mathbf{r}_j \mathbf{r}_k \mathbf{r}_m} \delta_{\mathbf{r}_m \mathbf{r}_i} \delta_{\mathbf{r}_m \mathbf{r}_j} \delta_{\mathbf{r}_m \mathbf{r}_k} \delta_{\mathbf{r}_m \mathbf{r}_l} \quad . \]  

(4.74)

Matrix elements involving \( H_c \) are much more tedious and can be found from Equations 4.67, 4.73, D9, and D10 as follows:

\[ \langle \mathbf{r}_i' \mathbf{r}_i ; \mathbf{r}_i' \mathbf{r}_m | H_c | \mathbf{r}_i \mathbf{r}_j \mathbf{r}_k \mathbf{r}_m \rangle = \frac{1}{2} \sum_{\mathbf{r}_i' \mathbf{r}_i' \mathbf{r}_m} \sum_{\mathbf{r}_i' \mathbf{r}_i' \mathbf{r}_m} C_{\mathbf{r}_i' \mathbf{r}_i} C_{\mathbf{r}_i' \mathbf{r}_m} C_{\mathbf{r}_i' \mathbf{r}_m} \]
\[ X \left[ \langle N'e's' \, \alpha' \, \beta' \, \gamma' \, \delta' \; K'IM \mid H_e \mid N's\gamma 'm \; KIM \rangle \\
+ (-)^2 X + \delta' \langle N'e's' \, \alpha' \, \beta' \, \gamma' \, \delta' \; -K'IM \mid H_e \mid N's\gamma 'm \; KIM \rangle \\
+ (-)^2 X + \delta' \langle N'e's' \, \alpha' \, \beta' \, \gamma' \, \delta' \; +K'IM \mid H_e \mid N's\gamma 'm \; KIM \rangle \right] \] (4.75)

\[ = \alpha, \, \hbar, \, \omega \sum (N'e's'\, \alpha' \, \beta' \, \gamma' \, \delta') (N's\gamma 'm) \sum (N'e's'\, \alpha' \, \beta' \, \gamma' \, \delta') (N's\gamma 'm) s_{KK'} s_{mm'} \left\{ \sum_{\ell=0}^{\infty} (\ell + \delta (\ell + 1) - 2 K m)^2 s_{KK'} s_{mm'} \\
+ (-)^2 \sum_{\ell=0}^{\infty} (\ell + \delta (\ell + 1) - 2 K m)^2 s_{KK'} s_{mm'} \right\} \phi (\ell, K) \phi (\ell, m) \\
- s_{KK'} s_{mm'} \phi (\ell, K) \phi (\ell, m) \] (4.76)

where

\[ \phi (\ell, m) = \sqrt{(\ell + \delta (\ell + 1) - 2 K m)^2} \quad m \leq \ell \]
\[ = 0 \quad m > \ell \] (4.77)

The quantities involving \( \phi (j, \pm m) \) and \( \phi (I, \pm K) \) arise by noting the analytic forms (121, p. 91) of the Clebsch-Gordan coefficients that occur in matrix elements of the form \( \langle K'IM \mid N'e's' j' m' I'j' \mid KIM \rangle \). Even though these matrix elements are elementary to solve, the calculation still requires considerable computer time because of the double sum over the spherical quantum numbers (N\&s\&jm). Therefore care must be taken not only in choosing the maximum size of the particle basis function, but also in deciding how many of the accessible energy levels will be allowed in the final calculations. The former determines how long the computer will take solving each matrix element while the latter is related to the number of matrix elements that must be determined before the diagonalization can take
place. The last three columns of Table 4.8 show the number of basis states that are allowed in the final diagonalization when the single-particle levels made accessible to the extra core nucleon are limited to (a) all levels with \( N \leq 5 \), (b) all levels with \( N \leq 3 \), and (c) only the lower three levels for each \( 1F \). The purpose of the table is merely to illustrate how the number of basis states increases with increasing \( I \), and so only the positive parity states with \( I \leq 5/2 \) are shown.

Figure 4.2 shows the final energy levels plotted as a function of the rotational parameter \( \alpha_1 \). The particle basis is truncated at the \( N=3 \) shell, and only the three lowest extra-core particle states are allowed for each nucleon. The parameters are chosen in such a way that when \( \alpha_1 = 0 \), the energy levels degenerate into the levels of Figure 4.1a with \( \beta_3 = 0.6 \). Figure 4.3 shows the experimental levels of \( ^{13}C \) and \( ^{13}N \) normalized to the theoretical energy scale parameter \( \hbar \omega \). A reasonable value for \( \hbar \omega \) can be obtained from the rule (107, p. 18)

\[
\hbar \omega \approx 4.1 A^{-\frac{1}{2}} \text{ MeV},
\]

where \( A \) is the atomic mass of the system. Inserting \( A = 13 \) into the last equation gives \( \hbar \omega \approx 17 \text{ MeV} \).

Notice that the ordering of the six lowest theoretical levels is in agreement with experiment when \( \alpha_1 \) is larger than 0.06. It was found that such agreement could be obtained whenever the lowest two accessible particle states were \( \Gamma_2 \) and \( \Gamma_1 \) respectively, with an energy difference of about 0.1\( \hbar \omega \). The energy spacing is not too good; however, this can be improved somewhat by varying the parameters as will be considered shortly.
Table 4.8. The values of $K$ and $J_i$ which are allowed in the coupled basis function of Equation 4.67 are tabulated for various values of $I^\pi$. Only positive parity states are shown with $I=\frac{3}{2}$. The last three columns show the number of basis states that occur when the single-particle levels accessible to the extra-core nucleon are limited to (a) all levels with $N \leq 5$, (b) all levels with $N \leq 3$, and (c) only the lower three levels of each IR. Also shown are the total number of basis states that must be used in the final diagonalization for each of the three cases.

<table>
<thead>
<tr>
<th>$I^\pi$</th>
<th>$K$</th>
<th>$J_i$</th>
<th>(a)</th>
<th>(b)</th>
<th>(c)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{1}{2}^+$</td>
<td>$\frac{1}{2}$</td>
<td>$1$</td>
<td>18</td>
<td>6</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Total number of basis states:</td>
<td>18</td>
<td>6</td>
</tr>
<tr>
<td>$\frac{3}{2}^+$</td>
<td>$\frac{1}{2}$</td>
<td>$1$</td>
<td>18</td>
<td>6</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Total number of basis states:</td>
<td>35</td>
<td>11</td>
</tr>
<tr>
<td>$\frac{5}{2}^+$</td>
<td>$\frac{1}{2}$</td>
<td>$1$</td>
<td>18</td>
<td>6</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Total number of basis states:</td>
<td>53</td>
<td>17</td>
</tr>
</tbody>
</table>
Figure 4.2. Final energy levels expressed in units of $\hbar \omega$ as a function of the rotational parameter $\alpha_1$. For simplicity, the levels are denoted by (21)$^\text{th}$. The particle parameters are $\beta_2=0.4$, $\beta_3=0.0$, $\kappa=0.075$, and $\mu=0.0$.

Figure 4.3. Experimental energy levels of $^{13}_N$ and $^{13}_C$ expressed as a function of the energy scale parameter $\hbar \omega$. Levels are again denoted by (21)$^\text{th}$. 
When the entire set of extra-core particle wavefunctions with $N \geq 3$ were included as accessible states for the last nucleon, it was found that all of the final energy levels were lowered by a small amount. Fortunately, the relative spacings of the levels were perturbed very little by this expanded basis, so that such calculations will not be considered further. Also, several computer runs were performed using all particle states less than $N=5$ in the particle Hamiltonian, but still limiting the accessible particle states in the last diagonalization to the three lowest ones for each IR. Since the number of particle bases states per IR is now 18 or 19 (instead of 6 or 7 for $N=3$), it takes the computer roughly $(19/7)^2 \approx 8$ times as long to calculate each matrix element. After considerable calculation, it was found that little or no improvement was obtained with this extended basis.

3. Calculating transition matrix elements

After the total Hamiltonian has been diagonalized, the final wavefunction will be of the form

$$|\Sigma M \eta; \varphi \rangle = \sum_{\Sigma \lambda} B_{\Sigma \lambda}^{\Sigma \eta \varphi} \sum_{(\pi \sigma \delta \varphi \eta \mu)} C_{\Sigma \lambda}^{\pi \sigma \delta \varphi \eta \mu}$$

$$\chi \left\{ |\pi \sigma \delta \varphi \eta \mu; \Sigma \lambda \rangle + (-)^{\pi - \delta} |\pi \sigma \delta \varphi \eta \mu; -\Sigma \lambda \rangle \right\}^{\Sigma \lambda}.$$

The theoretical reduced transition matrix elements are then of the form
where the reduced matrix elements inside the curly brackets for the various operators can be obtained from Equations 4.48 through 4.56.

In the last part of this section, various reduced matrix elements among the lowest four energy levels will be calculated and compared with experiment. Because of the quadruple sum in Equation 4.80, some of the reduced matrix elements will involve finding around 2000 individual terms. However, such a computation presents no difficulty because the transition matrix elements are calculated only once after the best agreement with the experimental energy levels has been obtained.

4. Results for the mass A=13 nuclei

The actual computer computations involved in the calculation can be conveniently summarized from the flow chart diagram of Figure 4.4. The boxed terms characterize individual computer programs that were written, while the quantities enclosed in square braces represent calculations which were transferred by cards to other programs. Finally, the information inside the curly brackets indicate the theoretical calculations which can be compared directly with experiment. Using such a procedure, one must first vary the parameters of the theory to obtain the best agreement possible between the theoretical and experimental energy levels. The validity of the model can then be further tested by using the resultant eigenvectors to
Figure 4.4. Flow chart showing actual method used in the calculations. Boxed terms represent individual computer programs, and the square-braced terms indicate card output which is fed into next program. Finally, the terms in the curly brackets represent theoretical results which can be compared with experiment.
compute various reduced matrix elements. These matrix elements can then also be compared with experiment.

The results for the mass A=13 system are encouraging, but somewhat inconclusive. Although five variables ($\hat{h}\omega, \alpha_1, \beta_2, \beta_3$, and $\chi$) were allowed in the calculation, we were unable to obtain excellent agreement with the experimental levels for any reasonable values of the parameters. However, quite good agreement with experiment could be obtained equally well with several different sets of variables. In some ways, this latter point is a desirable trait of the model, because it implies that the actual number of independent parameters is less than five. It also offers a distinct disadvantage, since it means that it is very difficult to find a unique point in the five parameter space which gives the optimum agreement with experiment. Thus, within the framework of the present model, the shape of the nuclear core will remain largely an indeterminant.

The number of genuine, independent parameters in the system can be found by a careful analysis of numerous final diagonalization curves such as the one shown in Figure 4.2. As has been mentioned before, the only definite criterion for obtaining good agreement with the eight lowest observed levels is that the energy separation between the two lowest particle levels accessible to the extra-core nucleon be approximately $0.10 \hat{h}\omega$. Such a separation distance can be produced in the particle Hamiltonian by a variety of parameters. In fact, any two of the three particle parameters ($\beta_2, \beta_3$, and $\chi$) can be arbitrarily chosen to have reasonable values, and the third can then be varied in order to produce the desired separation distance. In addition, a degenerate relation also occurs among the last two variables $\alpha_1$ and $\hat{h}\omega$, as can be seen by comparing Figures 2.2 and 2.3.
So, in reality, only two of the parameters need to be varied in order to obtain good agreement with experiment.

Although Nilsson (107) used $\lambda=0.05$ for the 1p and 2s-1d shell in his original paper, more recent calculations (122-124) indicate that a value of $\lambda=0.08$ may be more realistic for nuclei in the 2s-1d shell. Still other authors have allowed $\lambda$ to vary considerably for different nuclei within the 2s-1d shell (125,126). Since the Nilsson model yields levels in poor agreement with experiment for much of the 1p shell, it is difficult to estimate what $\lambda$ should be from past calculations. A reasonable estimate, however, can be derived from the observed energy separation of the $P_\frac{3}{2}$ and $P_\frac{1}{2}$ states in high energy p-p scattering from $^{16}O$. Such experimental data (127) indicate that the $P_\frac{3}{2}$ and $P_\frac{1}{2}$ states are bound with energies of 12.4 and 19.0 MeV respectively. If one considers $^{16}O$ to be a spherical nucleus, the energy separation, 6.6 MeV, may be attributed entirely to the spin-orbit splitting.

From Equation 3.30, we find that the relevant equation for this case is

$$3\lambda \hbar\omega = \Delta E = 6.6 \text{ MeV} \quad (4.81)$$

Taking $\hbar\omega=16.5$ MeV, which can be shown from Equation 4.78 to be appropriate for $^{16}O$, we find that the spin-orbit parameter is $\lambda=0.134$. In the present work, we shall limit our value of $\lambda$ to 0.15.

The first calculations were attempted by arbitrarily choosing $\hbar\omega$ and to be 17 MeV and 0.15 respectively, and allowing the parameter $\beta_3$ to vary in steps of 0.1 between 0.0 to 0.8. The final two parameters, $\beta_2$ and $\alpha_1$, were then varied to obtain the optimum agreement with the experiment levels. The best agreement was achieved with $\beta_3=0.4$, $\beta_2=-0.50$, and $0.05 \leq \alpha_1 \leq 0.06$ as is shown in Figure 4.5. Another set of parameters which gave nearly as good
Figure 4.5. The experimental levels of $^{13}$C and $^{13}$N are compared to the theoretical levels of the UAP model when $\hbar \omega$ is arbitrarily chosen to be 17 and 12 MeV respectively. The levels are again denoted by $2I^\pi$. 
results was $\beta_3=0.5$, $\beta_2=-0.42$, and $0.05 \leq \gamma \leq 0.06$. In order to see how sensitive the agreement was with different energy parameters, we next arbitrarily chose $\hbar \omega$ to be 12 MeV, and carried out the same fitting procedure. Again good agreement was obtained for $0.4 \leq \beta_3 \leq 0.06$, and the best set of parameters was found to be $\beta_2=-0.38$, $\beta_3=0.5$, and $0.075 \leq \gamma \leq 0.085$ (as also shown in Figure 4.5). Both sets of theoretical curves agree about equally well with experiment.

The fitting procedures were done by visual means. A chi-squared fit would be impractical in the present calculations for several reasons, such as:

1. The model has five parameters, and we could easily have introduced three more. A chi-squared fit to such a problem, considering the computer time involved, would have been prohibitive.

2. Interactions not included in the model (such as pairing effects, alpha correlations, particle-hole couplings, vibrations of the core, etc.) would be expected to perturb the levels somewhat. Such corrections in the theoretical level spectrum could render a chi-squared fit useless.

3. Other approximations were introduced after the Hamiltonian had already been formulated. For example, the particle basis states were truncated at the $N=3$ oscillator shell, and only the three lowest particle states accessible to the extra nucleon were allowed in the final diagonalization program.

4. At least eight experimental levels would have had to have been used in the fitting procedure, and a weighting factor would have had to have been assigned to each of these levels.
Because of these difficulties involved in the chi-squared fitting procedure, it would be almost impossible to decide which of the two theoretical energy curves in Figure 4.5 is the more physical from energy considerations alone. A more realistic approach to the problem would be to compare the theoretical reduced matrix elements with the corresponding experimental quantities. Table 4.9 shows various experimental gamma decay widths among the four lowest states of $^{13}\text{C}$ and $^{13}\text{N}$ which were taken from two review articles (44,128). Nearly all of the higher lying states decay by particle emission. The last two columns show the reduced transition probability which can be calculated by means of Equations 4.9, 2.81, and 2.82.

The reduced matrix elements were calculated for the four sets of parameters shown in Table 4.10. The energy levels for all four sets of parameters are drawn in Figure 4.4. For completeness, we shall also present the eigenvectors for the four lowest theoretical states which are used in the calculations. From Figure 4.4, we see that these levels have $I^P = \frac{1}{2}^-$, $\frac{1}{2}^+$, $2^-$, and $5^+$ respectively. From Equations 4.67 and 4.79, we see that the final wavefunctions can be written as

$$| \Psi_M \rangle = \sum_{\lambda, s}^{\lambda = 0, s = \frac{1}{2}} C_{\lambda, s} \Psi_{\lambda, s} | \lambda, s \rangle$$

where

$$| \Psi_{\lambda, s} \rangle = \frac{1}{\sqrt{2}} \sum_{\lambda = 1, \lambda = 1}^{\lambda = 0, \lambda = 0} C_{\lambda, s} \left[ | \lambda, s \rangle M \right]_{\lambda, s}$$

In analogy to Equations 3.39 and 3.40, we note that the coefficients in the last equation may also be expressed as

$$| \Psi_{\lambda, s} \rangle = \sum_{\lambda = 1, \lambda = 1}^{\lambda = 0, \lambda = 0} C_{\lambda, s} | \lambda, s \rangle M$$
Table 4.9. Reduced transition probabilities and reduced matrix elements for the mirror nuclei $^{13}\text{C}$ and $^{13}\text{N}$. Experimental data for $^{13}\text{C}$ is shown above dotted line and $^{13}\text{N}$ data is below the line.

<table>
<thead>
<tr>
<th>Initial state $(L^F\text{-MeV})$</th>
<th>Final state $(L^F\text{-MeV})$</th>
<th>Type of transition</th>
<th>Width (ev)</th>
<th>Reduced transition probability $(e^2 \text{ fm}^2$ or $\mu^2 \text{ fm}^2$)</th>
<th>Reduced transition probability (Meissner units)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{1+}\frac{3}{2} -3.086$</td>
<td>$^{1-}\frac{1}{2} -0.0$</td>
<td>E1</td>
<td>$0.44\pm0.04$</td>
<td>$(2.9\pm0.4)10^{-3}$</td>
<td>$0.0143\pm0.0013$</td>
</tr>
<tr>
<td>$^{3-}\frac{3}{2} -3.684$</td>
<td>$^{1+}\frac{1}{2} -3.086$</td>
<td>E1</td>
<td>$(3.3\pm1.2)10^{-5}$</td>
<td>$0.0064\pm0.0023$</td>
<td>$0.018\pm0.006$</td>
</tr>
<tr>
<td>$^{3-}\frac{3}{2} -3.684$</td>
<td>$^{1+}\frac{1}{2} -3.086$</td>
<td>E2</td>
<td>$(8.4\pm3.2)10^{-7}$</td>
<td>$3.90\pm1.48$</td>
<td>$2.05\pm1.78$</td>
</tr>
<tr>
<td>$^{5+}\frac{5}{2} -3.55$</td>
<td>$^{1-}\frac{1}{2} -0.0$</td>
<td>M2</td>
<td>$(5.9\pm2.0)10^{-5}$</td>
<td>$7.80\pm2.64$</td>
<td>$0.861\pm0.291$</td>
</tr>
<tr>
<td>$^{1+}\frac{3}{2} -2.366$</td>
<td>$^{1-}\frac{1}{2} -0.0$</td>
<td>E1</td>
<td>$0.45\pm0.05$</td>
<td>$(7.9\pm4.7)10^{-7}$</td>
<td>$111.0\pm66.0$</td>
</tr>
<tr>
<td>$^{3-}\frac{3}{2} -2.37$</td>
<td>$^{1+}\frac{1}{2} -2.37$</td>
<td>E1</td>
<td>$0.035$</td>
<td>$1.025\pm0.036$</td>
<td>$0.092\pm0.10$</td>
</tr>
<tr>
<td>$^{1-}\frac{1}{2} -2.37$</td>
<td>$^{1+}\frac{1}{2} -2.37$</td>
<td>M1</td>
<td>$0.65$</td>
<td>$0.0226$</td>
<td>$0.0638$</td>
</tr>
<tr>
<td>$^{5+}\frac{5}{2} -3.55$</td>
<td>$^{1-}\frac{1}{2} -0.0$</td>
<td>M2</td>
<td>$&lt; 2.0\times10^{-3}$</td>
<td>$&lt; 398.5$</td>
<td>$&lt; 43.0$</td>
</tr>
</tbody>
</table>
Table 4.10. Various sets of parameters which yield energy states in good agreement with experiment.

<table>
<thead>
<tr>
<th>$\beta_2$</th>
<th>$\beta_3$</th>
<th>$\kappa$</th>
<th>$\Delta \omega$ (MeV)</th>
<th>$\alpha_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>-0.38</td>
<td>0.5</td>
<td>0.15</td>
<td>12</td>
<td>0.075</td>
</tr>
<tr>
<td>-0.38</td>
<td>0.5</td>
<td>0.15</td>
<td>12</td>
<td>0.085</td>
</tr>
<tr>
<td>-0.50</td>
<td>0.4</td>
<td>0.15</td>
<td>17</td>
<td>0.050</td>
</tr>
<tr>
<td>-0.50</td>
<td>0.4</td>
<td>0.15</td>
<td>17</td>
<td>0.060</td>
</tr>
</tbody>
</table>
The coefficients therefore depend only on the particle parameters, and they are tabulated in Tables 4.11 and 4.12 for the two sets of particle parameters given in Table 4.10. The coefficients $B_{\alpha,\kappa,\lambda}$ are also tabulated in Tables 4.13 and 4.14. The reduced matrix elements can now be calculated in a straightforward manner, as has been previously described.

The observed values for the magnetic dipole moments of $^{13}$C and $^{13}$N are

$$\mu_{1/2}^Z = (0.702381 \pm 0.000002) \mu_N$$

and

$$\mu_{1/2}^- = -(0.32212 \pm 0.00035) \mu_N$$

respectively. The theoretical values for these quantities are found from Equations 4.11, 4.12, 4.17, 4.19, and 4.30. The result is

$$\mu_{1/2}^Z = \left( \begin{array}{cc} 0 & 0 \\ 1 & 0 \end{array} \right) \mathcal{M}_{z} + \left( \begin{array}{cc} 0 - g_s - g_c \end{array} \right) \mu_e + \left( g_s - g_c \right) \mu_{1/2}^z$$

which simplifies in the present case to

$$\mu_{1/2}^Z = \frac{1}{2} \left\{ \mu_e + (g_s - g_c) \mu_{1/2}^z + (g_s - g_c) \mu_{1/2}^z \right\}$$

Remembering that $g_c = 1/2$ and that $g_L$ and $g_S$ are given in Equations 4.20 and 4.21, we find that the theoretical magnetic dipole moments are

$$\mu_{1/2}^Z = \frac{1}{2} \left\{ 0.500 < \mu_e > + 0.500 < \mu_L > - 3.8 \mu_e < \mu_s > \right\}$$

for $^{13}$C, and
Table 4.11. The coefficients $C(N_{2s}\ell j m)$ are tabulated for the three lowest extra-core particle states of each IR when the particle parameters $\beta_2=-0.38, \beta_3=0.5, \text{ and } \gamma=0.15$. For clarity, the spherical quantum numbers are expressed as $N, \ell, 2j, \text{ and } 2m$. The constant value of $S=1/2$ is not included.

<table>
<thead>
<tr>
<th>N</th>
<th>$\ell$</th>
<th>2j</th>
<th>2m</th>
<th>($r_1$, 1)</th>
<th>($r_1$, 2)</th>
<th>($r_1$, 3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0.1692</td>
<td>-0.0059</td>
<td>-0.0427</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>5</td>
<td>1</td>
<td>0.5445</td>
<td>-0.6973</td>
<td>-0.2335</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>3</td>
<td>1</td>
<td>0.1388</td>
<td>0.3942</td>
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<tr>
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<td>1</td>
<td>1</td>
<td>0.6413</td>
<td>0.3771</td>
<td>0.4907</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>7</td>
<td>7</td>
<td>-0.4236</td>
<td>-0.3177</td>
<td>0.6947</td>
</tr>
<tr>
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<td>3</td>
<td>7</td>
<td>-5</td>
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<td>-0.3313</td>
<td>0.4151</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>5</td>
<td>-5</td>
<td>0.1695</td>
<td>0.0741</td>
<td>0.2184</td>
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<table>
<thead>
<tr>
<th>($r_2$, 1)</th>
<th>($r_2$, 2)</th>
<th>($r_2$, 3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>5</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>7</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>5</td>
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<td>3</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>($r_3$, 1)</th>
<th>($r_3$, 2)</th>
<th>($r_3$, 3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>5</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>7</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>5</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>3</td>
</tr>
</tbody>
</table>
Table 4.12. The coefficients $C_{ij}^{(N_{S}j_{m})}$ are tabulated for the three lowest extra-core particle states of each IR when the particle parameters are $\beta_2=-0.50$, $\beta_3=0.4$, and $x=0.15$.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$\ell$</th>
<th>$2j$</th>
<th>$2m$</th>
<th>$(\Gamma_1, 1)$</th>
<th>$(\Gamma_1, 2)$</th>
<th>$(\Gamma_1, 3)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0.1679</td>
<td>-0.0107</td>
<td>-0.0338</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>5</td>
<td>1</td>
<td>0.5323</td>
<td>-0.6687</td>
<td>-0.2455</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>3</td>
<td>1</td>
<td>0.1472</td>
<td>0.3766</td>
<td>0.2679</td>
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<tr>
<td>2</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0.6642</td>
<td>0.2339</td>
<td>-0.5259</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>7</td>
<td>7</td>
<td>-0.4178</td>
<td>-0.4854</td>
<td>0.7280</td>
</tr>
<tr>
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<td>3</td>
<td>7</td>
<td>-5</td>
<td>-0.1658</td>
<td>-0.3470</td>
<td>0.1079</td>
</tr>
<tr>
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<td>3</td>
<td>5</td>
<td>-5</td>
<td>0.1537</td>
<td>0.0110</td>
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<table>
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<th>$N$</th>
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<th>$2j$</th>
<th>$2m$</th>
<th>$(\Gamma_2, 1)$</th>
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<tr>
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<td>-5</td>
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<th>$(\Gamma_3, 2)$</th>
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<td>2</td>
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<td>3</td>
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<tr>
<td>3</td>
<td>3</td>
<td>5</td>
<td>-3</td>
<td>0.0474</td>
<td>0.1534</td>
<td>0.0215</td>
</tr>
<tr>
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<td>3</td>
<td>-3</td>
<td>0.2012</td>
<td>-0.4732</td>
<td>0.6201</td>
</tr>
</tbody>
</table>
Table 4.13. The coefficients $B^{[\Pi]}_{\frac{1}{2}, \alpha} K$ are tabulated for the four lowest states (denoted by $I^\pi$) for two values of the rotational parameters $\alpha_1$. The other parameters are $\beta_2 = -0.38$, $\beta_3 = 0.5$, and $\chi = 0.15$. The values for $Q$ and $K$ are not given since $Q = 1$ for the four states of interest, and the values for $K$ can be found from Table 4.8. The eigenvectors do not depend upon $\pi_0$.

| $(I^-_1, \alpha_1)$ | $\alpha_1 = 0.075$ | | $\alpha_1 = 0.085$ | |
|---------------------|-------------------|-------------------|
|                     | $\frac{1^-}{2}$   | $\frac{1^+}{2}$   | $\frac{3^-}{2}$   | $\frac{5^+}{2}$   | $\frac{1^-}{2}$   | $\frac{1^+}{2}$   | $\frac{3^-}{2}$   | $\frac{5^+}{2}$   |
| $(I^-_1, 1)$        | 0.0               | 0.9754            | 0.0               | 0.5888            | 0.0               | 0.9691            | 0.0               | 0.5678            |
| $(I^-_1, 2)$        | 0.0               | 0.1507            | 0.0               | -0.2247           | 0.0               | 0.1706            | 0.0               | -0.2421           |
| $(I^-_1, 3)$        | 0.0               | 0.1611            | 0.0               | -0.0259           | 0.0               | 0.1780            | 0.0               | -0.0351           |
| $(I^-_2, 1)$        | 0.9172            | 0.0               | 0.9720            | -0.3935           | 0.9092            | 0.0               | 0.9692            | -0.3771           |
| $(I^-_2, 2)$        | 0.3974            | 0.0               | 0.2111            | 0.4315            | 0.4152            | 0.0               | 0.2208            | 0.4471            |
| $(I^-_2, 3)$        | 0.0298            | 0.0               | 0.0500            | 0.0299            | 0.0315            | 0.0               | 0.0557            | 0.0331            |
| $(I^-_3, 1)$        | 0.0               | 0.0               | 0.0887            | 0.5013            | 0.0               | 0.0               | 0.0913            | 0.5147            |
| $(I^-_3, 2)$        | 0.0               | 0.0               | -0.0175           | 0.0889            | 0.0               | 0.0               | -0.0208           | 0.0926            |
| $(I^-_3, 3)$        | 0.0               | 0.0               | 0.0026            | -0.0321           | 0.0               | 0.0               | 0.0045            | -0.0365           |
Table 4.14. The coefficients $B_{\frac{1}{2}, \frac{1}{2}}^{\ell, \alpha_1}$ are tabulated for the four lowest states (denoted by $I^\pi$) for two values of the rotational parameter $\alpha_1$. The other parameters are $\beta_2=-0.50, \beta_3=0.4$, and $\chi=0.15$. Again, the redundant values for $Q$ and $K$ are not given.

<table>
<thead>
<tr>
<th>$(\ell, \alpha_1)$</th>
<th>$\alpha_1=0.050$</th>
<th>\phantom{1}</th>
<th>$\alpha_1=0.060$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\frac{1^-}{2}$</td>
<td>$\frac{1^+}{2}$</td>
<td>$\frac{3^-}{2}$</td>
</tr>
<tr>
<td>$(1^-_1, 1)$</td>
<td>0.0</td>
<td>0.9819</td>
<td>0.0</td>
</tr>
<tr>
<td>$(1^-_1, 2)$</td>
<td>0.0</td>
<td>0.0513</td>
<td>0.0</td>
</tr>
<tr>
<td>$(1^-_1, 3)$</td>
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<td>0.1825</td>
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<tr>
<td>$(1^-_2, 1)$</td>
<td>0.8761</td>
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</tr>
<tr>
<td>$(1^-_2, 2)$</td>
<td>0.4814</td>
<td>0.0</td>
<td>0.3094</td>
</tr>
<tr>
<td>$(1^-_2, 3)$</td>
<td>0.0260</td>
<td>0.0</td>
<td>0.0464</td>
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<tr>
<td>$(1^-_3, 1)$</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0840</td>
</tr>
<tr>
<td>$(1^-_3, 2)$</td>
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<td>0.0</td>
<td>-0.0103</td>
</tr>
<tr>
<td>$(1^-_3, 3)$</td>
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<td>0.0</td>
<td>0.0063</td>
</tr>
</tbody>
</table>
From Equations 4.89, 4.52, 4.54, and 4.55, we can show that the magnetic dipole moments (as well as M1 transitions) do not have a direct dependence on the core deformation parameters ($\beta_2$ or $\beta_3$). In addition, they are independent of the energy parameter $\hbar\omega$. Consequently, a comparison of the theoretical dipole moment with experiment should be a good test of the ground state eigenvector. Such a comparison is made in Table 4.15 for the four sets of parameters given in Table 4.10. For completeness, the single particle shell model prediction is also given. The necessary formula for the shell model is simply

$$\mu_{1/2}^- = \sqrt{\frac{1}{6}} \left\{ 0.500 < \| \tilde{L} || > + 0.500 < \| \tilde{L} \| > + 4.856 < \| \tilde{J} || > \right\} \quad (4.91)$$

for $^{13}\text{N}$.

Another experimental quantity which is caused by the magnetic dipole operator is the M1 transition between the $\frac{3^-}{2}$ and $\frac{1^-}{2}$ states. The
Table 4.15. The magnetic dipole moments of $^{13}\text{C}$ and $^{13}\text{N}$ are calculated for the four different sets of parameters given in Table 4.10 as well as for the single particle shell model. All numbers are in units of the nuclear magneton $\mu_N$.

<table>
<thead>
<tr>
<th></th>
<th>$\langle \frac{1}{2} | \frac{1}{2} | \frac{1}{2} \frac{1}{2} \rangle$</th>
<th>$\langle \frac{1}{2} | \frac{1}{2} | \frac{1}{2} \frac{1}{2} \rangle$</th>
<th>$\langle \frac{1}{2} | \frac{1}{2} | \frac{1}{2} \frac{1}{2} \rangle$</th>
<th>$\langle \frac{1}{2} | \frac{1}{2} | \frac{1}{2} \frac{1}{2} \rangle$</th>
<th>$^{13}\text{C}$</th>
<th>$^{13}\text{N}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experimental</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>0.70238</td>
<td>-0.32212</td>
</tr>
<tr>
<td>Shell Model</td>
<td>---</td>
<td>1.2247</td>
<td>1.6330</td>
<td>-0.40825</td>
<td>0.63767</td>
<td>-0.26433</td>
</tr>
<tr>
<td>$\hbar\omega=12$ MeV</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\alpha=0.075$</td>
<td>1.22474</td>
<td>0.50623</td>
<td>0.91448</td>
<td>-0.40825</td>
<td>0.78433</td>
<td>-0.41099</td>
</tr>
<tr>
<td>$\alpha=0.085$</td>
<td>1.22474</td>
<td>0.53095</td>
<td>0.93920</td>
<td>-0.40825</td>
<td>0.77929</td>
<td>-0.40595</td>
</tr>
<tr>
<td>$\hbar\omega=17$ MeV</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\alpha=0.050$</td>
<td>1.22474</td>
<td>0.38728</td>
<td>0.79553</td>
<td>-0.40825</td>
<td>0.80861</td>
<td>-0.43528</td>
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<tr>
<td>$\alpha=0.060$</td>
<td>1.22474</td>
<td>0.43221</td>
<td>0.84046</td>
<td>-0.40825</td>
<td>0.79944</td>
<td>-0.42611</td>
</tr>
</tbody>
</table>
Experimental reduced matrix elements for this transition can be calculated directly from Table 4.9 using Equation 4.10. The values are

\[ |\langle \frac{1}{2}^- | M(i) | \frac{1}{2}^- \rangle | = (1.75 \pm 0.08) \mu_N \]  

(4.93)

for $^{13}\text{C}$, and

\[ |\langle \frac{1}{2}^- | M(i) | \frac{1}{2}^- \rangle | = 1.6 \mu_N \]  

(4.94)

for $^{13}\text{N}$. Since the operator $I$ does not contribute to $M1$ transitions, the theoretical formulas are simply

\[ |\langle \frac{1}{2}^- | M(i) | \frac{1}{2}^- \rangle | = | -0.500 \langle \frac{1}{2}^- | J \cdot L | \frac{1}{2}^- \rangle | - 3.826 \langle \frac{1}{2}^- | E \cdot L | \frac{1}{2}^- \rangle | \]  

(4.95)

and

\[ |\langle \frac{1}{2}^- | M(i) | \frac{1}{2}^- \rangle | = | 0.500 \langle \frac{1}{2}^- | J \cdot L | \frac{1}{2}^- \rangle | + 4.586 \langle \frac{1}{2}^- | E \cdot L | \frac{1}{2}^- \rangle | \]  

(4.96)

for $^{13}\text{C}$ and $^{13}\text{N}$ respectively. The results are tabulated in Table 4.16. The error is roughly 12 percent for $^{13}\text{C}$ and 50 percent for $^{13}\text{N}$. Contrary to the results of the magnetic dipole moment, the parameters for $\hbar\omega=17$ MeV give slightly better agreement with experiment than those for $\hbar\omega=12$ MeV.

We shall next consider the various $E1$ transitions that have been observed among these states. The reduced matrix elements of these transitions that have been measured are given at the top of Table 4.17. Fortunately, the electric dipole moment of the core is zero, and the transition is produced entirely from the particle operator. In addition, the magnitude of the effective charge for the extra nucleon is $\frac{1}{2} e$ for both $^{13}\text{C}$ and $^{13}\text{N}$, and therefore the UAP model can predict the $E1$ transitions for these two nuclei at the same time (as shown in Table 4.17). One final calculation that is presented is the shell model prediction to $\langle \frac{1}{2}^+ | E(2) | \frac{3}{2}^- \rangle$ assuming that the states involved are pure $2s\frac{1}{2}$ and $1p\frac{1}{2}$ single-particle states respectively.
Table 4.16. The quantity $\langle \frac{3}{2} - \| m(3) \| \frac{1}{2} \rangle$ is calculated for the four sets of parameters given in Table 4.10 and compared with experiment.

<table>
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<tr>
<th>$\hbar \omega$</th>
<th>$\langle \frac{3}{2} - | m(3) | \frac{1}{2} \rangle$</th>
<th>$\langle \frac{3}{2} - | m(3) | \frac{1}{2} \rangle$</th>
<th>$\langle \frac{3}{2} - | m(3) | \frac{1}{2} \rangle$</th>
<th>$^{13}$C</th>
<th>$^{13}$N</th>
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<tr>
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<td>---</td>
<td>---</td>
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<td>1.61</td>
</tr>
<tr>
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<tr>
<td>$\alpha_1$=0.075</td>
<td>0.46356</td>
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<td>2.43</td>
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<tr>
<td>$\alpha_1$=0.085</td>
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<td>-0.58006</td>
<td>1.98</td>
<td>2.43</td>
</tr>
<tr>
<td>$\hbar \omega$=17 MeV</td>
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<td></td>
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<td></td>
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<tr>
<td>$\alpha_1$=0.050</td>
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<td>2.36</td>
</tr>
<tr>
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<td>0.50823</td>
<td>1.07983</td>
<td>-0.57160</td>
<td>1.93</td>
<td>2.37</td>
</tr>
</tbody>
</table>
Table 4.17. Comparison of theoretical El reduced matrix element with experiment. Also shown are the predictions of the shell model for $\langle 1/2^+ | E(1) | 1/2^- \rangle$ with various choices for $\hbar \omega$. All numbers are given in units of $\text{e fm}$.

|                  | $\langle 1/2^+ | E(0) | 1/2^- \rangle$ | $\langle 1/2^- | E(1) | 1/2^+ \rangle$ | $\langle 5/2^- | E(1) | 3/2^+ \rangle$ |
|------------------|-----------------|-----------------|-----------------|
| **Experiment**   |                 |                 |                 |
| $^{13}\text{C}$  | 0.169±0.008     | 0.228±0.015     | 0.196±0.038     |
| $^{13}\text{N}$  | 0.255±0.015     | 0.30            | ---             |
| **Single-particle shell model** |          |                 |                 |
| $\hbar \omega=12$ MeV | 0.371           | ---             | ---             |
| $\hbar \omega=17$ MeV | 0.312           | ---             | ---             |
| $\hbar \omega=22$ MeV | 0.274           | ---             | ---             |
| **Single-particle estimate** | 0.84            | 1.19            | 1.45            |
| **UAP model**    |                 |                 |                 |
| $\hbar \omega=12$ MeV |               |                 |                 |
| $\alpha_1=0.075$ | 0.2676          | 0.0591          | 0.3336          |
| $\alpha_1=0.085$ | 0.2700          | 0.0606          | 0.3308          |
| $\hbar \omega=17$ MeV |               |                 |                 |
| $\alpha_1=0.050$ | 0.2350          | 0.0420          | 0.2306          |
| $\alpha_1=0.060$ | 0.2405          | 0.0455          | 0.2380          |
for various values of $\hbar \omega$. Also shown is the single-particle estimate calculated from Equation 2.81. The large discrepancy between this value and the other shell model calculations shows that the single-particle estimates to the reduced transition probabilities (Equations 2.81 and 2.82) are sometimes off by a factor of ten or more, and must not be taken too seriously. Again, there is considerable variance between the theoretical and experimental reduced matrix elements. The discrepancy is the greatest for the quantity $\langle \frac{3}{2} \| E(1) \| \frac{1}{2} \rangle$, where the theoretical values are smaller than experiment by a factor of four or five. However, a similar situation has been shown to exist in the Hartree-Fock shell model (130). The theoretical value of $\langle \frac{3}{2} \| E(1) \| \frac{1}{2} \rangle$ is in this case underestimated by a factor of three from experiment. It should also be noticed that the observed reduced matrix elements of $^{13}$N are somewhat larger than the corresponding ones of $^{13}$C. The difference is usually attributed to the fact that the extra-core nucleon in $^{13}$N has a larger rms radius due to the additional coulomb repulsion from the core (131).

Finally, we shall consider the three higher order electric transitions which have been measured for $^{13}$C (c.f. Table 4.9). The experimental reduced matrix elements for these three decays are given in the top row of Table 4.18. For such transitions, the effective charge of the extra-core neutron is extremely small (104, p. 334), and so to a very good approximation we can assume the decay to be caused entirely from the intrinsic electric moments of the core. These moments are related to the deformation parameters by Equation 4.25 which is

\[
E_{\alpha, \nu}^C = \frac{\frac{3}{2} Z e R_0 \hat{\alpha}}{\sqrt{4\pi (2\alpha + 1)}} \mathcal{A}_{\alpha, \nu}^b .
\]  

(4.97)
Table 4.18. The theoretical reduced matrix elements for three electric transitions of $^{13}\text{C}$ are compared with the corresponding experimental quantities. Also shown are the intrinsic quadrupole and octopole moments for various sets of parameters which are needed in the calculations.

|                  | $E_{20}^c$ (fm$^2$) | $E_{33}^c$ (fm$^3$) | $\langle \frac{3}{2}^+|E(2)|\frac{1}{2}^-\rangle$ (e fm$^2$) | $\langle \frac{5}{2}^+|E(2)|\frac{1}{2}^-\rangle$ (e fm$^2$) | $\langle \frac{5}{2}^+|E(3)|\frac{1}{2}^-\rangle$ (e fm$^3$) |
|------------------|---------------------|---------------------|--------------------------------------------------|--------------------------------------------------|--------------------------------------------------|
| Experimental     | ---                 | ---                 | 5.13$^{+0.27}_{-0.29}$                             | 4.83$^{+0.85}_{-1.02}$                            | 25.8$^{+6.8}_{-8.4}$                              |
| $\hbar\omega=12$ MeV |                     |                     |                                                  |                                                  |                                                  |
| $\lambda_1=0.075$ | 9.97                | 37.70               | 9.13                                             | 3.00                                             | 6.79                                             |
| $\lambda_2=0.085$ | 9.97                | 37.70               | 9.50                                             | 2.63                                             | 10.32                                            |
| $\hbar\omega=17$ MeV |                     |                     |                                                  |                                                  |                                                  |
| $\lambda_1=0.050$ | 9.26                | 17.88               | 9.12                                             | 2.58                                             | 2.15                                             |
| $\lambda_2=0.060$ | 9.26                | 17.88               | 9.41                                             | 2.43                                             | 0.91                                             |
The parameter $R_0$ is the effective radius of the surface and is defined by Equations 4.23 and 4.24. If the nucleons are in a harmonic oscillator potential, one can show from theoretical arguments (49, p. 469) that $R_0$ is related to the energy parameter, $\hbar \omega$, by the approximate equation

$$R_0^2 = \frac{5B}{\hbar \omega [\text{MeV}]} m^2$$

(4.98)

For heavy nuclei, one finds $R_0 = 1.2A^{1/3} \text{ fm}$, and by inserting this value into the previous equation, one obtains $\hbar \omega = 4A^{-1/3} \text{ MeV}$ as was noted earlier (c.f. Equation 4.78). From the last two equations, we can now calculate the theoretical intrinsic moments for the four sets of parameters of Table 4.9, and these values are given in the first two columns of Table 4.18. The other three columns compare the theoretical values for the three reduced matrix elements with experiment. The first quantity is predicted too high by about 80 percent for all four sets of parameters, and the second one is consistently too low by a factor of two. The prediction for the octopole reduced matrix element is also too small. However, unlike all other matrix elements considered, its theoretical value varies by a factor of ten among the four sets of parameters used.

The results of the UAP model are therefore quite satisfactory in that the lowest eight experimental levels, as well as some of the low-lying transitions, seem to be reasonably well predicted. It is quite disappointing, however, that we could not find a unique set of parameters which give optimum agreement with the experimental energy levels and reduced matrix elements.
5. Comparison with other models

The mass $A=13$ nuclei have been studied extensively within the framework of several different models. Two papers on the intermediate coupling shell model were carried out over fifteen years ago and were found to give fair agreement with the observed negative parity states (132). The positive parity states have also been treated successfully by both the strong-coupling Nilsson model (133) and the weak-coupling collective model (134).

The results of the UAP model presented in the present work seem to have a definite advantage over the above mentioned models since the energies of both negative and positive parity states are well-predicted with one set of parameters. However, recent Hartree-Fock calculations on the mass $A=13$ nuclei (130,135) have also succeeded in correlating most of the low-lying energy levels with experiment. The reduced matrix elements predicted with this model are in no better agreement with experiment than those of the UAP model. As noted earlier, both models predict a value for $\langle \frac{3}{2}^+ | E(1) | \frac{1}{2}^+ \rangle$ which is at least a factor of three smaller than experiment. Such a coincidence may indicate that the two models are more similar than one would first expect.

F. Possible Applications of the UAP Model to Other Nuclei

The previous two sections have shown that the UAP model very likely has some validity for the $A=9$ and $A=13$ mass systems. The model can be easily extended to the mass $A=17$, 21, and 25 nuclei where the $\alpha$-cluster core would presumably have $T_d$, $D_{2d}$, and $D_{2h}$ symmetries respectively. The $A=25$ calculation would be very similar to previous calculations that have been done by Chi et al. (121,124,125) on the asymmetric rotor. The primary
difference would be in the values used for the rotational parameters $A^K$. From our calculations on $^{24}\text{Mg}$, we would expect the core Hamiltonian of the $A=25$ nuclei to have two variable rotational parameters, $A_j$ and $A^2$, with $A^2 > A_j$. However, Chi assumed only one variable among these parameters by restricting the ratios of the rotational parameters to be those of the hydrodynamic estimate as given in Equation 3.11.

As has already been mentioned, the UAP model runs into some additional complications when it is applied to the assumed $T_d$ symmetry of the $A=17$ mass nuclei. Nevertheless, the coupled wavefunctions can be constructed by projection operator techniques and making explicit use of Equation B15. It should be noted, however, that at least two alpha model calculations (136, 137) have been attempted on $^{17}_0$. The calculations differ from the present model in that the Hamiltonian is diagonalized among a "weakly-coupled" basis as described in Equation 3.44. Such a basis has a definite advantage in that one does not need to work with double-valued groups. However, one main problem of this approach is that it is impossible to truncate the particle states in the manner described in the present work. If one were to repeat the calculation in the "strongly-coupled" basis used in the present work, the results could be quite different.
V. CONCLUSIONS

The primary objective of this thesis has been to obtain further evidence for $\alpha$-clustering in light nuclei by means of investigating two different types of phenomenological $\alpha$-particle models. The CAP model, which was considered for all $A=4N$ nuclei below $^{40}$Ca, was found to be quite successful in predicting a variety of properties among the low-lying energy states. For all nuclei above $^{16}$O, several plausible $\alpha$-structures existed for each nucleus, and we had to choose the correct structure from the experimental data. The CAP model thus has an additional degree of freedom not found in other collective models. One might argue that the apparent success of the CAP model is therefore due merely to this additional variable not found in other models. However, it is the somewhat optimistic, but firm belief of the present author that this additional freedom is physical, and that some light even-even nuclei do indeed have varied molecular shapes. The other model considered was the UAP model which also yielded quite satisfactory results for the mass $A=9$ and $A=13$ nuclei. Unfortunately, in the latter case, the theoretical levels and reduced matrix elements were rather insensitive to the parameters used, and it was therefore impossible to determine an accurate shape for these nuclei.

For both models, it is found that the positions of the energy states are usually well predicted by theory, but that the theoretical reduced matrix elements quite often differ from experiment by a factor of two or more. A possible explanation for this fact is that the positions of the energy levels are largely determined by the symmetry of the structure, while the transition rates depend more on the exact nature of the eigenvector.
During the course of this work, several unsolved problems have arisen which would seem to warrant immediate investigation. One of these problems involves the application of various cluster model calculations on the $D_{2d}$ distorted tetrahedron and $D_{2h}$ bitetrahedron $\alpha$-structures for $^{20}\text{Ne}$ and $^{24}\text{Mg}$. The procedures for such calculations were briefly mentioned in Section IIIJ. The other calculation was suggested in Section IIIG, where it was stated that the 4-body calculation of $^{16}\text{O}$ could be done by diagonalizing the realistic $\alpha$-particle Hamiltonian among translationally invariant harmonic oscillator states. The procedure for constructing such states is given in the literature (138), and the analogous 4-body nucleon problem of $^4\text{He}$ has already been done (139,140). Since both of these calculations are fairly straightforward, it would not be surprising if one or both of these problems were attempted within the next few years.
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VIII. APPENDICES

A. Rotation Matrices

Throughout this thesis, the notation used in performing rotations of angular momentum wavefunctions is identical to that of Rose (25), but different from most other standard texts (41, 104, 141, 142). Rotations on the wavefunctions will be defined in the active sense, that is

\[ O_R \Psi_{\pm m}(x) = \Psi_{\pm m}(Rx) \quad (A1) \]

However, rotations on the vector \( \mathbf{x} \) will be carried out passively, so that we leave the vector fixed and rotate the coordinate system. Such a rotation requires three variables, and in the present work we consider these variables to be three Euler angles which were explicitly defined in Figure 2.1.

With these definitions, one can show in a straightforward manner that

\[ \langle \mathbf{x}' | \hat{J}_m \rangle = \sum_{m'} D_{m',m}^{\hat{J}}(\alpha, \beta, \gamma) \langle \mathbf{x} | \hat{J}_m' \rangle \quad (A2) \]

and conversely

\[ \langle \mathbf{x} | \hat{J}_m \rangle = \sum_{m'} D_{m,m'}^{\hat{J}^*}(\alpha, \beta, \gamma) \langle \mathbf{x}' | \hat{J}_m' \rangle \quad (A3) \]

where \( r \) and \( r' \) are defined in the laboratory and rotated coordinated systems respectively. The explicit form for the matrix elements of the rotation matrix \( D^{\hat{J}}(R) \) is

\[ D_{m',m}^{\hat{J}}(\alpha, \beta, \gamma) = e^{-i m' x} d_{m',m}^{\hat{J}}(\beta) e^{-i m y} \quad (A4) \]

where

\[ d_{m',m}^{\hat{J}}(\beta) = \frac{(-1)^m}{(\hat{J} + m)! (\hat{J} - m)!} \frac{1}{(\hat{J} + m')! (\hat{J} - m')!} \]
If the angular momenta $\mathbf{j}$ are limited to integral values, the wavefunctions $|j m\rangle$ generate IR's of the rotation group in three dimensions, $R(3)$, and $D^j(R)$ is a matrix representation of the rotation $R$ for the IR labeled by $j$. In general, however, $j$ can be either integral or half-integral, and so the wavefunctions generate IR's of $SU_2$, the special unitary group in two dimensions.

For later use, we shall also note the group property of these rotations. We define $R$ and $S$ as passive rotations on the coordinate system such that

$$R \mathbf{x} = \mathbf{x}'$$

$$S \mathbf{x}' = \mathbf{x}''$$

so that

$$(s R) \mathbf{x} = \mathbf{x}'' .$$

By repeated usage of Equations A1 and A2, we then note

$$O_S O_R <\nu | \hat{d} \hat{m}'> = O_S <\nu' | \hat{d} \hat{m}'> = \sum_{m'} D_{m m'}^\dagger (s) D_{m' m'}(R) <\nu' | \hat{d} \hat{m}' >$$

Also, from Equation A7,

$$O_S O_R <\nu | \hat{d} \hat{m}'> = <\nu'' | \hat{d} \hat{m}'> = \sum_{m} D_{m m''}^\dagger (s R) <\nu'' | \hat{d} \hat{m} > .$$

Combining Equation A8 and A9, we find the desired result which is

$$D_{m m''}^\dagger (s R) = \sum_{m'} D_{m' m''}^\dagger (R) D_{m m'}(s) .$$
B. Rotation Properties of Wavefunctions

In Chapters II and IV, we showed that the eigenstates of the Hamiltonian for many collective and unified models could be expanded in terms of the wavefunctions $D^{LR}_{M,L,L}(\alpha,\beta,\gamma)$ and $D^{IK}_{M,L,L}(\alpha,\beta,\gamma)$ respectively. Consequently, it becomes necessary to consider the effects on these wavefunctions of various rotations carried out in the body-fixed coordinate system which leave the Hamiltonian invariant.

Any structure which is a symmetric or asymmetric rotor is spatially invariant under only two types of rotations, these being:

1. $C_z^z(\phi)$—an arbitrary rotation of angle $\phi$ about the body-fixed $z$ axis, and

2. $C_x^{xy}(\phi)$—a rotation of $180^\circ$ about an axis in the $xy$ plane that subtends an angle $\phi$ from the body-fixed $x$ axis.

By carefully examining Figure 2.1, we see that these rotations alter the Euler angles in the following way:

$$C_z^z(\phi); \quad (\alpha, \beta, \gamma) \rightarrow (\alpha, \beta, \gamma + \phi) \quad (B1)$$

and

$$C_2^{xy}(\phi); \quad (\alpha, \beta, \gamma) \rightarrow (\alpha + \pi, \pi - \beta, 2\pi - \gamma - 2\phi) \quad (B2)$$

Since the rotations were carried out in $R(3)$ space, the changes of the Euler angles could have been written in other ways. For example, the $2\pi$ could have been omitted from the last equation. However, for wavefunctions of half integer $j$, a rotation of $2\pi$ is not the identity operation, and omission of $2\pi$ in this case would imply a different operation. Therefore, Equation (B2) uniquely defines the operation $C_x^{xy}(\phi)$ in the $SU_2$ group, although this was not the original intent.
In carrying out the operations, we make use of the equations
\[ D^\prime_{m',m} (\alpha, \beta, \gamma) = e^{i m' \phi} D^\prime_{m',m} (\beta) e^{-i m \gamma} \]  
\[ (B3) \]
and
\[ d^{\prime}_{m',m} (\pi, -\beta) = (\pi^{\prime} m', \pi^{\prime}, -\pi^{\prime}) d^{\prime}_{m',-m} (\beta). \]  
\[ (B4) \]
Equation B3 follows directly from Equation A4. The last equation can be obtained indirectly from Equation A5 and noting that (141, p. 60)
\[ d^{\prime}_{m',m} (\pi, -\beta) = c_{m'} c^{-1}_{m'} (\pi) d^{\prime}_{m, m'} (\pi, -\beta). \]  
\[ (B5) \]
From Equations B1, B2, B3, and B4, one can then show:
\[ C_z^z (\phi) D^z_{m, K} (\alpha, \beta, \gamma) = e^{-i m \phi} D^z_{m, K} (\alpha, \beta, \gamma) \]  
\[ (B6) \]
\[ C_z^{xy} (\phi) D^{xy}_{m, K} (\alpha, \beta, \gamma) = e^{-i \pi \phi} e^{2 \pi i m \phi} D^{xy}_{m, K} (\alpha, \beta, \gamma) \]  
\[ (B7) \]
Similarly, one can show
\[ C_z^z (\phi) D^z_{m, K} (\alpha, \beta, \gamma) = e^{-i m \phi} D^z_{m, K} (\alpha, \beta, \gamma) \]  
\[ (B8) \]
\[ C_z^{xy} (\phi) D^{xy}_{m, K} (\alpha, \beta, \gamma) = e^{-i \pi \phi} e^{2 \pi i m \phi} D^{xy}_{m, K} (\alpha, \beta, \gamma) \]  
\[ (B9) \]
The rotation of the body-fixed particle wavefunctions can be obtained from Equation A2 and noting that these operations, which are carried out in the body-fixed coordinates, do not affect the particle wavefunctions in the laboratory coordinates, \( \langle r | j m \rangle \) (104, p. 257). With Equations B3 and B9, one then finds
\[ C_z^z (\phi) \langle r' | j m \rangle = e^{-i m \phi} \langle r' | j m \rangle \]  
\[ (B10) \]
\[ C_z^{xy} (\phi) \langle r' | j m \rangle = e^{-i \pi \phi} e^{2 \pi i m \phi} \langle r' | j, -m \rangle \]  
\[ (B11) \]
For spherical top rotors, the structures are spatially invariant under additional rotations about axes that are skew to the xy plane. For these rotations, the formulas for the change in Euler angles (such as Equations B1 and B2) are very complicated, and it is much easier to work with the matrix representations of these body-fixed rotations which can be found by taking the complex conjugate of Equation A10

\[ D_{M'K'}^x (A) = \sum_{K'} D_{K'M'}^x (S) D_{M'K'}^x (A) \]  \hspace{1cm} (B12)

The rotation \( R \) now represents the three usual Euler angles that specify the orientation of the body-fixed axes, and \( S \) is the additional operation carried out in the body-fixed coordinate system. The elements of the matrix representations for the two rotations considered earlier are (c.f. Figure B1)

\[ c^{xz} (\phi): \hspace{1cm} D_{K'M'}^z (\alpha, \beta, \phi) = S_{K'M'} \in \mathbb{C} \]  \hspace{1cm} (B13)

and

\[ c^{xy} (\phi): \hspace{1cm} D_{K'M'}^y (\alpha, \beta, \pi - 2\phi) = S_{K'M'} \in \mathbb{C} \]  \hspace{1cm} (B14)

By combining Equations B13 and B14 with Equation B12, one obtains Equation B6 and B7 as expected.

One example of a rotation which would warrant explicit usage of Equation B12 is the \( C_3 \) rotation in the tetrahedral group (c.f. Figure 2.4). As shown in Figure B2, this rotation cyclically permutes the three body-fixed axes, and is equivalent to the Euler angles \((S_1, S_2, S_3) = (0, \pi/2, \pi/2)\). We therefore find

\[ \tilde{c}_{3}^{\gamma z} D_{M'K'}^x (\alpha, \beta, \gamma) = \sum_{K'} D_{K'M'}^x (\alpha, \beta, \gamma) D_{M'K'}^x (\alpha, \beta, \gamma) \]  \hspace{1cm} (B15)
Figure B1. Schematic showing that the rotation $C^Z_{X Y}(\phi)$ is equivalent to the three Euler rotations $(S_1, S_2, S_3) = (0, \pi, \pi - 2\phi)$.

Figure B2. Schematic demonstrating the equivalence of $C^X_{Y Z}$ with the three Euler rotations $(S_1, S_2, S_3) = (0, \pi/2, \pi/2)$. 
C. Angular Momentum Coupling Relations

The derivation of many of the formulas in Chapter II and IV require an extensive use of Racah algebra, so it will be advantageous for us to summarize the more common relations in a separate appendix. The following identities are taken from numerous sources (25,42,142,143, pp. 1053-1068; 109, pp. 1-28), and no attempt will be made at present to justify their exact form.

The coupling of two angular momentum wavefunctions can be written as

\[
\langle \ell, \ell' | j, m \rangle = \sum_{m_1, m_2} C(\ell, \ell' | j, m_1, m_2, m) \langle \ell, \ell', m_1 \rangle \langle \ell', j, m_2 \rangle \langle \ell, j, m \rangle. \tag{C1}
\]

The coefficient on the right side of the equation is the usual Clebsch-Gordan coefficient that results from the reduction of tensor product of two IR's of SU2. The unitarity conditions of these coefficients are expressed as

\[
\sum_{m_1, m_2} C(\ell, \ell' | j, m_1, m_2, m) C(\ell, \ell' | j, m_1, m_2, m') = \delta_{j_1 j_2} \delta_{m m'} \tag{C2}
\]

and

\[
\sum_{j, m} C(\ell, \ell' | j, m_1, m_2, m) C(\ell, \ell' | j, m_1, m_2', m) = \delta_{m_1 m} \delta_{m_2 m_2'} \tag{C3}
\]

The Clebsch-Gordan coefficients are related to the 3-J symbol of Wigner by

\[
C(\ell, \ell' | j, m_1, m_2, m) = (-)^{\ell - \ell'} \sqrt{2 \ell + 1} \binom{\ell}{m_1, m_2, m} \tag{C4}
\]

The "3-J" symbols have easily recalled symmetry properties and are therefore usually preferred over Clebsch-Gordan coefficients in involved calculations. These symmetries are demonstrated in the next three equations which show the symmetry relations under (a) even permutation of columns.
(b) odd permutation of columns, and (c) simultaneous reversal of signs on
all three magnetic quantum numbers:

\[
\begin{pmatrix}
\hat{\mathbf{d}}_1 & \hat{\mathbf{d}}_2 & \hat{\mathbf{d}}_3 \\
m_1 & m_2 & m_3
\end{pmatrix}
= \begin{pmatrix}
\hat{\mathbf{d}}_1 & \hat{\mathbf{d}}_2 & \hat{\mathbf{d}}_3 \\
m & m_1 & m_2
\end{pmatrix}
= (-)^{m_1+m_2+m_3} \begin{pmatrix}
\hat{\mathbf{d}}_2 & \hat{\mathbf{d}}_1 & \hat{\mathbf{d}}_3 \\
m_1 & m & m_2
\end{pmatrix} \tag{C5}
= (-)^{m_1+m_2+m_3} \begin{pmatrix}
\hat{\mathbf{d}}_1 & \hat{\mathbf{d}}_2 & \hat{\mathbf{d}}_3 \\
-m_1 & -m_2 & -m_3
\end{pmatrix} .
\]

The unitarity conditions on the 3-J symbols are

\[
\sum_{m,m_2} \left( \begin{pmatrix}
\hat{\mathbf{d}}_1 & \hat{\mathbf{d}}_2 & \hat{\mathbf{d}}_3 \\
m & m_1 & m_2
\end{pmatrix} \begin{pmatrix}
\hat{\mathbf{d}}'_1 & \hat{\mathbf{d}}'_2 & \hat{\mathbf{d}}'_3 \\
m' & m'_1 & m'_2
\end{pmatrix} \right) = \frac{\delta_{m'm} \delta_{m_2m_2'}}{2 \hat{\mathbf{d}} + 1} \tag{C6}
\]

and

\[
\sum_{\hat{\mathbf{d}}} (2 \hat{\mathbf{d}}+1) \left( \begin{pmatrix}
\hat{\mathbf{d}}_1 & \hat{\mathbf{d}}_2 & \hat{\mathbf{d}}_3 \\
m & m_1 & m_2
\end{pmatrix} \begin{pmatrix}
\hat{\mathbf{d}}'_1 & \hat{\mathbf{d}}'_2 & \hat{\mathbf{d}}'_3 \\
m' & m'_1 & m'_2
\end{pmatrix} \right) = \delta_{m,m'} \delta_{m_2m_2'} . \tag{C7}
\]

The product of two rotation matrices with the same Euler angles can be ex­
pressed as

\[
D_{m_1,m_1'}(\alpha) D_{m_2,m_2'}(\alpha) = \sum_{\hat{\mathbf{d}} \hat{\mathbf{d}}} (2 \hat{\mathbf{d}}+1) D_{m_1,m_2}^\hat{\mathbf{d}}(\alpha) D_{m_1',m_2'}^\hat{\mathbf{d}}(\alpha) \tag{C8}
\]

This equation can be inverted using the orthogonality of the 3-J symbols to
yield

\[
\sum_{\hat{\mathbf{d}} \hat{\mathbf{d}}} D_{m_1,m_1}^\hat{\mathbf{d}}(\alpha) D_{m_2,m_2}^{\hat{\mathbf{d}}'}(\alpha) = \frac{\delta_{\hat{\mathbf{d}} \hat{\mathbf{d}}'}}{2 \hat{\mathbf{d}} + 1} D_{m_1,m_1'}(\alpha) \tag{C9}
\]

The rotations matrices are orthogonal in all their indices over inte­
gration of all 3 Euler angles, and one can write

\[
\int d\alpha D_{m_1,m_1'}(\alpha) D_{m_2,m_2}^{\hat{\mathbf{d}}'} = \frac{8 \pi^2}{2 \hat{\mathbf{d}} + 1} \delta_{\hat{\mathbf{d}} \hat{\mathbf{d}}'} \delta_{m_1,m_1'} \delta_{m_2,m_2} , \tag{C10}
\]

where

\[
\int d\alpha \equiv \int_0^{2\pi} d\alpha \int_0^\pi \sin \beta \ d\beta \int_0^{2\pi} d\gamma = 8 \pi^2 . \tag{C11}
\]
The last two equations can be combined to yield

$$\int d\mathbf{\alpha} D_{m' m}^{m} (\mathbf{1}) D_{m'' m}^{m} (\mathbf{1}) = 8 \pi^2 \left( \begin{array}{ccc} \hat{a}_1 & \hat{a}_2 & \hat{a}_3 \\ \hat{a}_1' & \hat{a}_2' & \hat{a}_3' \end{array} \right) \left( \begin{array}{ccc} \hat{m}_1 & \hat{m}_2 & \hat{m}_3 \\ \hat{m}_1' & \hat{m}_2' & \hat{m}_3' \end{array} \right).$$  \tag{C12}

Using the relation

$$\gamma_{\ell m} (\theta, \phi) = \sqrt{\frac{2\ell + 1}{4\pi}} D_{\ell m}^{\ell} (\theta, \phi),$$  \tag{C13}

one can develop some useful equations of spherical harmonics which are analogues of Equations C8, C9, C10, and C12. These are respectively

$$\gamma_{\ell m} (\theta, \phi) Y_{\ell m}^{\ell} (\theta, \phi) = \sqrt{\frac{2\ell + 1}{4\pi}} \left( \begin{array}{ccc} \ell & \ell & \ell \\ 0 & 0 & 0 \end{array} \right) \left( \begin{array}{ccc} \ell & \ell & \ell \\ m & m & m \end{array} \right) \gamma_{\ell m} (\theta, \phi),$$  \tag{C14}

$$Y_{\ell m}^{\ast} (\theta, \phi) \sqrt{\frac{(2\ell + 1)(2\ell + 1)}{4\pi}} \left( \begin{array}{ccc} \ell & \ell & \ell \\ 0 & 0 & 0 \end{array} \right) = \gamma_{\ell m} (\theta, \phi) \gamma_{\ell m} (\theta, \phi),$$  \tag{C15}

$$\int d\mathbf{\alpha} Y_{\ell m} (\theta, \phi) Y_{\ell' m'} (\theta, \phi) Y_{\ell m} (\theta, \phi) = \sqrt{\frac{(2\ell + 1)(2\ell' + 1)(2\ell + 1)}{4\pi}} \left( \begin{array}{ccc} \ell & \ell & \ell \\ m & m & m \end{array} \right) Y_{\ell' m} (\theta, \phi).$$  \tag{C16}

The last equation arises quite frequently in Chapter IV where various tensor matrix elements are evaluated. One additional formula which is needed for calculating matrix elements of magnetic operators is the gradient identity which can be expressed as

$$\nabla \omega \left( \gamma_{\ell m} \right) = (-)^K \sqrt{K} \gamma_{(2K+1)} (\gamma_{K}) (-)^{m\ell} \left( \omega \gamma_{m} \gamma_{m} \right) \gamma_{K-1, m}.$$  \tag{C17}

A very useful relation among tensor matrix elements is the Wigner-Eckart theorem which can be written as (42)

$$\langle \lambda' \lambda' \lambda' | T_{\ell m} | \lambda \lambda \lambda \rangle = (-)^{m' + \ell - \ell'} \gamma_{\ell' m'} \gamma_{\ell m} \gamma_{\ell' m} \gamma_{\ell m} \gamma_{\ell m}.$$  \tag{C18}

The last term of this equation is independent of magnetic quantum numbers and is referred to as the reduced matrix element. The tensor operator, $T_{\ell m}$, rotates in the same way as do angular momentum wavefunctions. So from
Equation A3, one has

$$T_{LM}^{(b)} = \sum_{M'} D_{M'M}^L (\alpha, \beta, \gamma) T_{LM'}^{(s)} ,$$  \hspace{1cm} (C19)

and conversely

$$T_{LM}^{(s)} = \sum_{M'} D_{M'M}^L (\alpha, \beta, \gamma) T_{LM'}^{(b)} ,$$  \hspace{1cm} (C20)

where (b) and (s) denote body-fixed and space-fixed coordinate systems respectively.

The Wigner 6-J symbol arises naturally in problems concerned with the coupling of three angular momenta. It is used extensively in the computation of reduced matrix elements, and is defined in terms of 3-J symbols as

$$\begin{array}{c}
\sum_{m_1, m_2, m_3} (-1)^{m_1 + m_2 + m_3 + \eta_1 + \eta_2 + \eta_3} (m_1 \ m_2 m_3) (\eta_1 \eta_2 \eta_3) (m_1 \ m_2 m_3) (\eta_1 \eta_2 \eta_3) (n_1 \ n_2 n_3) (\eta_1 \eta_2 \eta_3) (n_1 \ n_2 n_3) (\eta_1 \eta_2 \eta_3),
\end{array}$$

(C21)

Some of its more useful symmetry properties include (a) invariance under interchange of columns, and (b) invariance under simultaneous interchange of any two numbers in the bottom row with the corresponding two numbers in the top row.

The orthogonality condition for the 6-J symbols can be written as

$$\sum_{\ell} (2\ell + 1)(2\ell + 1) \left\{ \begin{array}{c}
\ell_1, \ell_2, \ell_3 \\
\ell, \ell, \ell
\end{array} \right\} \left\{ \begin{array}{c}
\ell_1, \ell_2, \ell_3 \\
\ell, \ell, \ell
\end{array} \right\} = \delta_\ell \delta'_{\ell'},$$  \hspace{1cm} (C22)

Two other special sum rules involving only 6-J symbols are

$$\sum_{\ell_3} (-1)^{\ell + \ell_3 + \ell_3} (2\ell_3 + 1) \left\{ \begin{array}{c}
\ell_1, \ell_2, \ell_3 \\
\ell, \ell_2, \ell_3
\end{array} \right\} \left\{ \begin{array}{c}
\ell_1, \ell_2, \ell_3 \\
\ell, \ell_2, \ell_3
\end{array} \right\} = \left\{ \begin{array}{c}
\ell_1, \ell_2, \ell_3 \\
\ell, \ell_2, \ell_3
\end{array} \right\} \left\{ \begin{array}{c}
\ell_1, \ell_2, \ell_3 \\
\ell_1, \ell_2, \ell_3
\end{array} \right\} ,$$  \hspace{1cm} (C23)

and

$$\sum_{\ell_3} (-1)^{s + \ell} (2\ell_3 + 1) \left\{ \begin{array}{c}
\ell_1, \ell_2, \ell_3 \\
\ell, \ell_2, \ell_3
\end{array} \right\} \left\{ \begin{array}{c}
\ell_1, \ell_2, \ell_3 \\
\ell, \ell_2, \ell_3
\end{array} \right\} = \sum_{\ell_3} (-1)^{s + \ell} (2\ell_3 + 1) \left\{ \begin{array}{c}
\ell_1, \ell_2, \ell_3 \\
\ell, \ell_2, \ell_3
\end{array} \right\} \left\{ \begin{array}{c}
\ell_1, \ell_2, \ell_3 \\
\ell, \ell_2, \ell_3
\end{array} \right\} ,$$  \hspace{1cm} (C24)
where
\[ S = f_1 + f_2 + f_3 + \ell_1 + \ell_2 + \ell_3 + \ell_1' + \ell_2' + \ell_3'. \]

Two other usual relations involve both 3-J and 6-J symbols; these are

\[
\sum_{m_3} \binom{\ell_1}{m_1} \binom{\ell_2}{m_2} \binom{\ell_3}{m_3} \binom{\ell_1'}{n_1} \binom{\ell_2'}{n_2} \binom{\ell_3'}{n_3} = \sum_{\ell_3 m_3} (-\ell_3^2 + m_3 + n_3 (2\ell_3 + 1)) \binom{\ell_1}{\ell_1} \binom{\ell_2}{\ell_2} \binom{\ell_3}{\ell_3} \binom{\ell_1'}{n_1} \binom{\ell_2'}{n_2} \binom{\ell_3'}{n_3} \tag{C25} \]

and

\[
\sum_{m_2 m_3} (-)^m_2 \binom{\ell_1}{m_1} \binom{\ell_2}{m_2} \binom{\ell_3}{m_3} \binom{-\ell_1}{-n_1} \binom{-\ell_2}{-n_2} \binom{-\ell_3}{-n_3} = \binom{\ell_1}{\ell_1} \binom{\ell_2}{\ell_2} \binom{\ell_3}{\ell_3} \binom{-\ell_1}{-n_1} \binom{-\ell_2}{-n_2} \binom{-\ell_3}{-n_3}, \tag{C26} \]

where
\[ S = \ell_1 + \ell_2 + \ell_3 + n_1 + n_2 + n_3. \]

The last equation yields a very useful identity for \( m_1 = m_2 = m_3 = 0 \) and \( \ell_3 = 1/2 \).

\[
\begin{pmatrix} \ell & \ell' & R \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell & \ell' & R \\ 0 & 0 & 0 \end{pmatrix} = -\frac{1 + (-)^{\ell_1 + \ell_3 + R}}{2 ((2\ell_3 + 1)(2\ell_3 + 1))} \begin{pmatrix} R & \ell' & \ell \\ 0 & \ell_3 & -\ell_3 \end{pmatrix}. \tag{C27} \]

We shall also make use of a 9-J symbol defined by Wigner to be

\[
\begin{pmatrix} f_{11} & f_{12} & f_{13} \\ f_{21} & f_{22} & f_{23} \\ f_{31} & f_{32} & f_{33} \end{pmatrix} = \sum_{\ell_3 m_3} (-)^{\ell_3} \binom{\ell_1}{\ell_1} \binom{\ell_2}{\ell_2} \binom{\ell_3}{\ell_3} \binom{\ell_1}{n_1} \binom{\ell_2}{n_2} \binom{\ell_3}{n_3} \binom{\ell_1'}{\ell_1'} \binom{\ell_2'}{\ell_2'} \binom{\ell_3'}{\ell_3'}. \tag{C28} \]

Symmetry properties of the 9-J symbol include (a) invariance under a reflection of the symbol about either diagonal, (b) invariance under even permutations of rows or columns, and (c) change in phase of \((-1)^S\), where \( S \) is the sum of all nine parameters, for odd permutation of rows and columns. Many relations exist between 9-J, 6-J and 3-J symbols. One relation that will be used in Chapter IV is
One final formula which is used in calculating matrix elements of magnetic operators is the gradient identity which is

\[ \nabla_\omega \left( r^K Y_{\ell K} \right) = (-)^{K-1} r^{K-1} \frac{Y_{K-1,\ell}}{r} \left( \omega_{\mu - \mu} - m \right) Y_{K-1,\ell} \]  

(D30)

D. Angular Momentum Operators

The cartesian components of the angular momentum operator, \( J_i \), have the following commutation relations in laboratory coordinates:

\[ [\hat{J}_i, \hat{J}_j] = \hat{J}_k = \frac{i}{2} \epsilon_{kij} \hat{J}_m \]  

(D1)

The components are defined in terms of pseudospherical coordinates as

\[ \hat{J}_\pm = \mp \sqrt{\frac{a}{2}} (\hat{x} \pm i \hat{y}) \]  

\[ \hat{J}_0 = \hat{J}_z . \]  

(D2)

They can be shown to satisfy the following equation

\[ \hat{J}_\nu |\hat{J}_m\rangle = \sqrt{\frac{2}{(\hat{J}_m + 1)}} \frac{\nu + 1}{\nu - \nu} \epsilon(\hat{J}_\nu; m, m') |\hat{J}_m\rangle . \]  

(D3)

For a rigid rotor, the space-fixed angular momentum operators thus operate on the symmetric top wavefunctions as

\[ L^{(s)} D_{mK}^{L*}(\alpha, \beta, \gamma) = \sqrt{\frac{l(l+1)}{4\pi}} \sum_{m'} C(LL; M, M') D_{mK}^{L*}(\alpha, \beta, \gamma) . \]  

(D4)
Angular momentum operators rotate as tensors of rank one. Therefore, using Equations C8, C19, and D4, as well as the symmetry and unitarity relations of the 3-J symbols, one can show that

\[ L^{(k)}_{\nu} \, D_{M'K'}^{L^*} (\kappa, \beta, \gamma) = (-)^{\nu \Omega (L + \Omega)} \sum_{M} c (L \Omega \Omega; \kappa, -\nu, K') \, D_{M'K'}^{L^*} (\kappa, \beta, \gamma). \]  

(D5)

A tedious calculation using Equations D2 and D5 would then show that the anticommutation relations hold for the cartesian components of \( \mathbf{L} \) in the body-fixed system, that is

\[ \left[ L^x, L_m \right] = -i \sum_{m} \epsilon_{xkm} L_m. \]  

(D6)

For odd-\( A \) nuclei, one must consider both the particle and total angular momenta (denoted \( j \) and \( I \) respectively). In space-fixed coordinates, one naturally has

\[ J^{(s)}_\nu D_{MN}^{I^*} (\kappa, \beta, \gamma) = \sqrt{\frac{4\pi}{(I + 1)}} \sum_{M'} c (I I I'; M_\mu M_\nu') \, D_{MN}^{I^*} (\kappa, \beta, \gamma) \]  

and

\[ \frac{\hat{\rho}}{\nu} | \hat{m}_s > = \sqrt{\frac{2}{I + 1}} \sum_{m_m} c (\hat{m}_s \hat{m}_s' ; m_\mu m_\nu') \, | \hat{m}_s' >. \]  

(D7)

The total angular momentum in the body-fixed frame will have the same form as Equation D5, that is

\[ J^{(k)}_\nu D_{MN}^{I^*} (\kappa, \beta, \gamma) = (-)^{\nu \Omega (I + 1)} \sum_{M'} c (I I I'; K, -\nu, K') \, D_{MN}^{I^*}. \]  

(D9)

However, the body-fixed angular momentum of the particle behaves the same as in the laboratory, as can be shown from Equations C19, D8, C8, and C2 as follows:

\[ \hat{m}_s' | \hat{m}_s > = \sum_{m_\mu m_\nu} D_{\hat{m}_s' \hat{m}_s}^{\hat{m}_s} D_{\hat{m}_s' \hat{m}_s'}, \left< \hat{m}_s' \right| \hat{m}_s. \]
Equations D9 and D10 are used in Chapter IV in evaluating matrix elements of the form

\[ \langle \kappa' \mu' \ell' \sigma' m' | H | \kappa \mu \ell \sigma m \rangle .\]

E. Single-Particle States of the Harmonic Oscillator

The single-particle Hamiltonian that is used in the present work is that of a three-dimensional spherical harmonic oscillator with spin-orbit coupling

\[ H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 r^2 + c \ell \cdot \xi . \]  

(E1)

Following Eder's notation (144, pp. 71-82), we rewrite the Hamiltonian as

\[ H = \kappa \omega \left[ -\frac{\sigma^2 + \rho^2}{2} + \frac{1}{2} \kappa \xi \ell \cdot \xi \right] , \]

(E2)

where \( \rho = r/r_o \), \( \kappa = -c/2 \hbar \omega \), and \( r_o \) is the oscillator length defined as \( r_o^2 = \hbar^2/m\omega^2 \).

The eigenvalues for the Hamiltonian are

\[ E = (N + \frac{3}{2}) \frac{\hbar}{2} \omega - \kappa \ell \omega \left[ \ell (\ell + 1) - \kappa (\kappa + 1) - s (s + 1) \right] , \]

(E3)

where the quantum numbers can have the following values:

\[ N = 0, 1, 2, 3, \ldots \]

\[ \ell = N, N-2, N-4, \ldots, 1, 0 \]
The eigenvectors can be decoupled in the usual way

\[ |\mathcal{N} \ell s j m\rangle = \sum_{m_s} C(s j \ell m \ell m_s) |\mathcal{N} \ell m_s \rangle |s m_s\rangle, \quad (E5) \]

where the orbital part is the product

\[ \langle \chi |\mathcal{N} \ell m_s \rangle = R_{\mathcal{N} \ell} (r) Y_{\ell m_s} (\theta, \phi). \quad (E6) \]

The radial wavefunction can be expressed analytically as

\[ R_{\mathcal{N} \ell} (r) = \sqrt{\frac{2 \eta!}{\gamma_0^{1/2} \Gamma(\eta + \ell + 3/2)}} r^\ell e^{-\frac{r}{2} \rho^2} L^{\ell + \frac{1}{2}}_{\eta} (\rho^2), \quad (E7) \]

where \( n \) is a redundant quantum number defined as \( 2n + \ell = N \), and the last term is the usual Laguerre polynomial which can be expressed in terms of Appell symbols as

\[ L^n_{\eta} (r) = \frac{1}{n!} \sum_{\rho=0}^{\infty} \frac{\left((-n - \ell, \rho)(\eta, \rho)\right)}{\rho!} (-r)^{\eta - \rho}. \quad (E8) \]

Most of the matrix elements evaluated in Chapter IV include the following radial integral:

\[ \langle N' \ell' | r^Q | N \ell \rangle = \int_0^\infty r^2 dr R_{N' \ell'} (r) r^Q R_{N \ell} (r) \]

\[ = 2 \sqrt{\frac{\eta! \eta'!}{\Gamma(\eta + \ell + 3/2) \Gamma(\eta + \ell' + 3/2)}} \gamma_0^Q \int_0^\infty d\rho R_{N' \ell'} (\rho) R_{N \ell} (\rho) \rho^{\eta + \ell + \frac{3}{2}}. \quad (E9) \]

The easiest way to evaluate such an integral on the computer for arbitrary \( N \) and \( \ell \) is to expand the radial wavefunctions by means of Equations E7 and E8 and evaluate the resultant integral by means of the identity...
\[ \int_0^\infty dt \ t^Q e^{-t} = \Gamma(Q+1). \quad (E10) \]

The final form can then be expressed as the following double sum

\[ \langle N' Q' | N Q | N' \rangle = (-)^{n+n'} \sqrt{\frac{n!}{n'!}} \frac{\Gamma(a+n'+\frac{1}{2}) \Gamma(a+n+\frac{1}{2})}{\gamma_0^Q} \]

\[ \times \sum_{p,p'} (-)^{p+p'} \frac{\Gamma(n'+n-p-q' + \frac{\ell + \ell + Q+1}{2})}{p! p'! (n'-p')! (n-p)! \Gamma(a'+\frac{1}{2}-n'-p') \Gamma(a+\frac{1}{2}-n-p)}. \quad (E11) \]